REVISITING RANDOM WALKS FOR LEARNING ON GRAPHS

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ABSTRACT

We revisit a recent model class for machine learning on graphs, where a random walk on a graph produces a machine-readable record, and this record is processed by a deep neural network to directly make vertex-level or graph-level predictions. We refer to these stochastic machines as **random walk neural networks (RWNNs)**, and through principled analysis, show that we can design them to be isomorphism invariant while capable of universal approximation of graph functions in probability. A useful finding is that almost any kind of record of random walk guarantees probabilistic invariance as long as the vertices are anonymized. This enables us, for example, to record random walks in plain text and adopt a language model to read these text records to solve graph tasks. We further establish a parallelism to message passing neural networks using tools from Markov chain theory, and show that over-smoothing in message passing is alleviated by construction in RWNNs, while over-squashing manifests as probabilistic under-reaching. We empirically demonstrate RWNNs on a range of problems, verifying our theoretical analysis and demonstrating the use of language models for separating strongly regular graphs where the 3-WL test fails, and transductive classification on arXiv citation network.

1 INTRODUCTION

Message-passing neural networks (MPNNs) are a popular class of neural networks on graphs where each vertex keeps a feature vector and updates it by propagating messages over neighbors (Battaglia et al., 2018). MPNNs have achieved success, one reason being their respect for the natural symmetries of graph learning problems, i.e., invariance to graph isomorphism (Chen et al., 2019). On the other hand, MPNNs in their basic form can be viewed as implementing color updates of the Weisfeiler-Lehman (1-WL) graph isomorphism test, and thus their expressive power is not stronger (Xu et al., 2019). Also, their inner working is often tied to the topology of the input graph, which is related to over-smoothing, over-squashing, and under-reaching of features under mixing (Giraldo et al., 2023).

In this work, we revisit an alternative direction for learning on graphs, where a random walk on a graph produces a machine-readable record, and this record is processed by a deep neural network that directly makes graph-level or vertex-level predictions. We refer to these stochastic machines as **random walk neural networks (RWNNs)**. Pioneering works were done in this direction, often motivated by the compatibility of random walks with sequence learning methods. Examples include DeepWalk (Perozzi et al., 2014) and node2vec (Grover & Leskovec, 2016) which use skip-gram on walks, AWE (Ivanov & Burnaev, 2018) which uses embeddings of anonymized walks (Micali & Zhu, 2016), and CRaWl (Tönshoff et al., 2023) which uses 1D CNNs on sliding window descriptions of walks. These methods were proven powerful in various contexts, such as graph isomorphism learning that require expressive powers surpassing 1-WL test (Tönshoff et al., 2023; Martinkus et al., 2023).

Despite the promises, unlike MPNNs, we currently have not reached a good principled understanding of RWNNs. First, in context of geometric DL, it is unclear how we can systematically incorporate the symmetries of graph learning problems into RWNNs, as their neural networks are not necessarily isomorphism invariant. Second, the upper bound of their expressive power, along with the requirements on each component to reach it, is not clearly known. Third, whether and how the over-smoothing and over-squashing problems may occur in RWNNs are not well understood. Addressing such questions is important, as they allow us to better understand the strengths and limits of the existing methods, and potentially design enhanced RWNNs by short-circuiting the search in their large design space.

Table 1: An overview of prior methods in context of RWNNs, and new components originating from our analysis. NB means non-backtracking; MDLR means minimum degree local rule (Section 2.1).

Method	Random walk	Recording function q	Reader NN f_θ
DeepWalk	Uniform	Identity	Skip-gram
node2vec	Second-order pq-walk	Identity	Skip-gram
AWE	Uniform	Anonymization	Embedding table
CRaWl	Uniform + NB	Sliding window	1D CNN
RW-AgentNet	Uniform	Neighborhoods	RNN
WalkLM	Uniform	Text attributes	Language model
Ours (Sections 2.1, 2.2, 3)	MDLR (+ NB) (2.1) (+ restarts) (2.2)	Anonymization (+ named neighborhoods) (2.1)	Any universal (3.1)

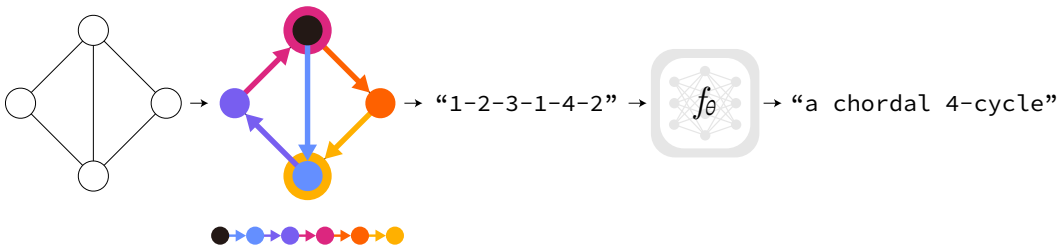

Figure 1: An RWNN that reads text record using a language model.

Contributions The main goal of our work is establishing a principled understanding of RWNNs with a focus on the aforementioned aspects. Our starting point is a new formalization of RWNNs which decouples random walks, their records, and neural networks that process them. This abstracts a wide range of design choices including prior methods, as in Table 1. The key idea of our analysis is then to understand RWNNs through a combination of two recent perspectives in geometric DL: probabilistic notions of invariance and expressive power (Bloem-Reddy & Teh, 2020; Abboud et al., 2021), and invariant projection of non-invariant neural networks (Puny et al., 2022; Dym et al., 2024).

This idea allows us to impose probabilistic invariance on RWNNs even if their neural networks lack symmetry, by instead requiring (probabilistic) invariance conditions on random walks and their records. This provides a justification for anonymized recording of walks (Micali & Zhu, 2016) and our novel extension of it using named neighborhoods. As long as probabilistic invariance holds, this also enables recording walks in plain text and adopting a language model to process them (Figure 1).

We then upper-bound the expressive power of RWNNs as universal approximation in probability which surpasses the WL hierarchy of MPNNs, under the condition that random walk records the graph of interest with a high probability. This establishes a useful link to cover times in Markov chains, providing guidance on designing random walks to minimize or bound the cover times. From this we motivate novel adaptation of minimum degree local rule (MDLR) walks (David & Feige, 2018) for RWNNs, and introduce restarts when working on a large and possibly infinite graph. We also provide a justification for the widespread use of non-backtracking (Tönshoff et al., 2023).

Continuing the link to Markov chain theory, we further analyze RWNNs and establish a parallelism to a linearized model of MPNNs. From this, we show that over-smoothing in MPNNs is inherently avoided in RWNNs, while over-squashing manifests as probabilistic under-reaching. This eliminates the typical trade-off between over-smoothing and over-squashing in MPNNs (Giraldo et al., 2023; Nguyen et al., 2023), and allows an RWNN to focus on overcoming under-reaching by scaling the walk length or using rapidly-mixing random walks such as non-backtracking walks.

We empirically demonstrate RWNNs on several graph problems. On synthetic setups, optionally with a small 1-layer transformer, we verify our claims on cover times, over-smoothing, and over-squashing. Then, we demonstrate adapting a language model (DeBERTa (He et al., 2021) to solve the challenging task of isomorphism learning of strongly regular graphs with perfect accuracy whereas the 3-WL test fails, improving over the previously known best result of RWNNs. We further suggest that our approach can turn transductive classification problem on a large graph into an in-context learning problem by recording labeled vertices during random walks. To demonstrate this, we apply Llama 3 (meta llama, 2024) model on transductive classification on arXiv citation network with 170k vertices, and show that it can outperform a range of MPNNs as well as zero- and few-shot baselines. Our experiments show the utility of our approach in analysis and development of RWNNs.

2 RANDOM WALK NEURAL NETWORKS

We start our discussion by formalizing random walk neural networks (RWNNs). We define an RWNN as a randomized function $X_\theta(\cdot)$ that takes a graph G as input and outputs a random variable $X_\theta(G)$ on the output space $\mathbb{R}^d$.[1] In case of vertex-level tasks, it is additionally queried with an input vertex v which gives a random variable $X_\theta(G, v)$. An RWNN consists of the following components:

1. **Random walk algorithm** that produces l steps of vertex transitions $v_0 \to \cdots \to v_l$ on the input graph G. If an input vertex v is given, we fix the starting vertex by $v_0 = v$.
2. **Recording function** $q : (v_0 \to \cdots \to v_l, G) \mapsto \mathbf{z}$ that produces a machine-readable record $\mathbf{z}$ of the random walk. It may access the graph G to record auxiliary information such as attributes.
3. **Reader neural network** $f_\theta : \mathbf{z} \mapsto \hat{\mathbf{y}}$ that processes record $\mathbf{z}$ and outputs a prediction $\hat{\mathbf{y}}$ in $\mathbb{R}^d$. It is the only trainable component and is not restricted to specific architectures.

For graph-level prediction, we sample $\hat{\mathbf{y}} \sim X_\theta(G)$ by running a random walk on G and processing its record using the reader NN f_θ. For vertex-level prediction $\hat{\mathbf{y}} \sim X_\theta(G, v)$, we query the input vertex v by simply starting the walk from it. In practice, we ensemble several sampled predictions e.g. by averaging, which can be understood as Monte Carlo estimation of the mean predictor $(\cdot) \mapsto \mathbb{E}[X_\theta(\cdot)]$.

We now analyze each component for graph-level tasks on finite graphs, and then vertex-level tasks on possibly infinite graphs. The latter simulates the problem of scaling to large graphs such as in transductive classification. As our definition captures many known designs (Table 1), we discuss them as well. We leave pseudocode in Appendix A.2 and leave notations and proofs in Appendix A.5.

2.1 GRAPH-LEVEL TASKS

Let $\mathbb{G}$ be the class of undirected, connected, and simple graphs[2]. Let $n \geq 1$ and $\mathbb{G}_n$ be the collection of graphs in $\mathbb{G}$ with at most n vertices. Our goal is to model a graph-level function $\phi : \mathbb{G}_n \to \mathbb{R}^d$ using an RWNN $X_\theta(\cdot)$. Since ϕ is a graph function, it is reasonable to assume isomorphism invariance:

$$\phi(G) = \phi(H), \quad \forall G \simeq H, \tag{1}$$

Incorporating the invariance structure to our model class $X_\theta(\cdot)$ would offer generalization benefit. As $X_\theta(\cdot)$ is randomized, we accept the probabilistic notion of invariance (Bloem-Reddy & Teh, 2020):

$$X_\theta(G) \overset{d}{=} X_\theta(H), \quad \forall G \simeq H. \tag{2}$$

A justification is that, if $X_\theta(\cdot)$ is invariant in probability, its mean predictor $(\cdot) \mapsto \mathbb{E}[X_\theta(\cdot)]$ would be an invariant function. For more in-depth discussion, please see Section 4. We now claim that we can achieve probabilistic invariance of $X_\theta(\cdot)$ by properly choosing the random walk algorithm and recording function while not imposing any constraint on the reader NN f_θ.

Proposition 2.1. *$X_\theta(\cdot)$ is invariant in probability, if its random walk algorithm is invariant in probability and its recording function is invariant.*

In other words, even if f_θ lacks symmetry, invariant random walk and recording function provably converts it into an invariant random variable $X_\theta(\cdot)$. This is an extension of invariant projection operators on functions (Puny et al., 2022; Dym et al., 2024) to a more general and probabilistic setup.

Random walk algorithm A random walk algorithm is invariant in probability if it satisfies:

$$\pi(v_0) \to \cdots \to \pi(v_l) \overset{d}{=} u_0 \to \cdots \to u_l, \quad \forall G \overset{\pi}{\simeq} H, \tag{3}$$

where $v_{[\cdot]}$ is a random walk on G, $u_{[\cdot]}$ is a random walk on H, and $\pi : V(G) \to V(H)$ specifies the isomorphism from G to H. It turns out that many random walk algorithms in literature are already invariant. To see this, let us write the probability of walking from a vertex u to its neighbor $x \in N(u)$:

$$\mathrm{Prob}[v_t = x | v_{t-1} = u] \coloneqq \frac{c_G(u, x)}{\sum_{y \in N(u)} c_G(u, y)}, \tag{4}$$

where the function $c_G : E(G) \to \mathbb{R}_+$ assigns positive weights (conductances) to edges. If we set $c_G(\cdot) = 1$, we recover uniform random walk used in DeepWalk (Perozzi et al., 2014). We show:

[1] While any output type such as text is possible (Figure 1), we explain with vector output for simplicity.

[2] We assume this for simplicity but extending to directed or attributed graphs is possible.

Proposition 2.2. *The random walk in Equation 4 is invariant in probability if its conductance $c_{[\cdot]}(\cdot)$ is invariant:*

$$c_G(u, v) = c_H(\pi(u), \pi(v)), \quad \forall G \overset{\pi}{\simeq} H. \tag{5}$$

It includes constant conductance, and any choice that only uses degrees of endpoints $\deg(u)$, $\deg(v)$.

We favor using degrees since it is cheap while potentially improving the behaviors of walks. Among many instantiations, we find that the following conductance function called the minimum degree local rule (MDLR) (Abdullah et al., 2015; David & Feige, 2018) is particularly useful:

$$c_G(u, v) \coloneqq \frac{1}{\min[\deg(u), \deg(v)]}. \tag{6}$$

MDLR is special as it has $O(n^2)$ vertex cover time, i.e., expected time of visiting all n vertices of a graph, optimal among first-order random walks (Equation 4) that use degrees of endpoints.

A common practice is to add non-backtracking property that enforces $v_{t+1} \neq v_{t-1}$ (Tönshoff et al., 2023), and we also find this beneficial. In Appendix A.1 we extend Equation 3 and Proposition 2.2 to second-order walks that include non-backtracking and node2vec walks (Grover & Leskovec, 2016).

Recording function A recording function $q : (v_0 \to \cdots \to v_l, G) \mapsto \mathbf{z}$ takes a random walk and produces a machine-readable record $\mathbf{z}$. We let $q(\cdot, G)$ have access to the graph G the walk is taking place. This allows recording auxiliary information such as vertex or edge attributes. A recording function is invariant if it satisfies the following for any given random walk $v_{[\cdot]}$ on G:

$$q(v_0 \to \cdots \to v_l, G) = q(\pi(v_0) \to \cdots \to \pi(v_l), H), \quad \forall G \overset{\pi}{\simeq} H. \tag{7}$$

Invariance requires that $q(\cdot, G)$ produces the same record $\mathbf{z}$ regardless of re-indexing of vertices of G into H. For this, we have to be careful in how we represent each vertex in a walk $v_0 \to \cdots \to v_l$ as a machine-readable value, and which auxiliary information we record from G. For example, identity recording used in DeepWalk (Perozzi et al., 2014) and node2vec (Grover & Leskovec, 2016) are not invariant as the result is sensitive to vertex re-indexing. We highlight two choices which are invariant:

- **Anonymization.** We name each vertex in a walk with a unique integer, starting from $v_0 \mapsto 1$ and incrementing it based on their order of discovery. For instance, a random walk $a \to b \to c \to a$ translates to a sequence $1 \to 2 \to 3 \to 1$.
- **Anonymization + named neighbors.** While applying anonymization for each vertex v in a walk, we record its neighbors $u \in N(v)$ if they are already named but the edge $v \to u$ has not been recorded yet. For instance, a walk $a \to b \to c \to d$ on a fully-connected graph translates to a sequence $1 \to 2 \to 3\langle 1\rangle \to 4\langle 1, 2\rangle$, where $\langle\cdot\rangle$ represents the named neighbors.

The pseudocode of both algorithms can be found in Appendix A.2. We now show the following:

Proposition 2.3. *A recording function $q : (v_0 \to \cdots \to v_l, G) \mapsto \mathbf{z}$ that uses anonymization, optionally with named neighbors, is invariant.*

While anonymization was originally motivated by privacy concerns in (Micali & Zhu, 2016) (also see Appendix A.6), Proposition 2.3 offers a new justification based on invariance. Our design of recording named neighbors is novel, and is inspired by sublinear algorithms that probe previously discovered neighbors in a walk (Dasgupta et al., 2014). In our context, it is useful since whenever a walk visits a set of vertices $S \subseteq V(G)$ it automatically records the entire induced subgraph $G[S]$. As a result, to record all edges of a graph, a walk only has to visit all vertices. While traversing all edges, i.e. edge cover time, is $O(n^3)$ (Zuckerman, 1991) in general, it is possible to choose a walk algorithm that takes only $O(n^2)$ time to visit all n vertices. MDLR in Equation 6 exactly achieves this.

Reader neural network A reader neural network $f_\theta : \mathbf{z} \mapsto \hat{\mathbf{y}}$ processes the record $\mathbf{z}$ of the random walk and outputs a prediction $\hat{\mathbf{y}}$ in $\mathbb{R}^d$. As in Proposition 2.1, there is no invariance constraint imposed on f_θ, and any neural network that accepts the recorded walks and has a sufficient expressive power can be used (we will make this precise in Section 3.1). This is in contrast to MPNNs where invariance is hard-coded in feature mixing operations. Also, our record $\mathbf{z}$ can take any format, such as a matrix, byte sequence, or plain text, as long as f_θ accepts it. Thus, it is possible (while not required) to choose the record to be plain text, such as `"1-2-3-1"`, and choose f_θ to be a pre-trained language model. This offers expressive power (Yun et al., 2020) and has a potential benefit of knowledge transfer from language domain (Lu et al., 2022; Rothermel et al., 2021).

2.2 VERTEX-LEVEL TASKS

We now consider vertex-level tasks. In case of finite graphs, we may simply frame a vertex-level task $(G, v) \mapsto \mathbf{y}$ as a graph-level task $G' \mapsto \mathbf{y}$ where G' is G with its vertex v marked. Then, we can solve $G' \mapsto \mathbf{y}$ by querying an RWNN $X_\theta(G, v)$ to start its walk at $v_0 = v$.

A more interesting case is when G is an infinite graph that is only locally finite, i.e. has finite degrees. This simulates problems on a large graph such as transductive classification. In this case, we may assume that our target function depends on finite local structures (Tahmasebi et al., 2023).

Let $r \geq 1$, and $\mathbb{B}_r \coloneqq \{B_r(v)\}$ be the collection of local balls in G of radius r centered at $v \in V(G)$. We would like to model a vertex-level function $\phi : \mathbb{B}_r \to \mathbb{R}^d$ on G using an RWNN $X_\theta(\cdot)$ by querying the vertex of interest, $X_\theta(G, v)$. We assume that ϕ is isomorphism invariant:

$$\phi(B_r(v)) = \phi(B_r(u)), \quad \forall B_r(v) \simeq B_r(u). \tag{8}$$

The probabilistic invariance of $X_\theta(\cdot)$ is defined as follows:

$$X_\theta(G, v) \overset{d}{=} X_\theta(G, u), \quad \forall B_r(v) \simeq B_r(u). \tag{9}$$

We can achieve probabilistic invariance by choosing the walk algorithm and recording function similar to the graph-level case[3]. As a modification, we query $X_\theta(G, v)$ with the starting vertex $v_0 = v$ of the random walk. Anonymization informs v to the reader NN by always naming it as 1.

Then, we make a key choice of localizing random walks with restarts. That is, we reset a walk to its starting vertex v_0 either with a probability $\alpha \in (0, 1)$ at each step or periodically every k steps. Restarting walks tend to stay more around starting vertex v_0, and were used to implement locality bias in personalized PageRank algorithm for search (Page et al., 1999). This localizing effect is crucial in our context since a walk can drift away from $B_r(v_0)$ before recording all necessary information, which may take an infinite time to return as G is infinite (Janson & Peres, 2012). Restarts make the return to v_0 mandatory, ensuring that $B_r(v_0)$ can be recorded in a finite expected time. We show:

Theorem 2.4. *For a uniform random walk on an infinite graph G starting at v, the vertex and edge cover times of the finite local ball $B_r(v)$ are not always finitely bounded.*

Theorem 2.5. *In Theorem 2.4, if the random walk restarts at v with any nonzero probability α or any period $k \geq r + 1$, the vertex and edge cover times of $B_r(v)$ are always finite.*

3 ANALYSIS

In Section 2, we have described the design of RWNNs, primarily relying on the principle of (probabilistic) invariance. In this section, we provide in-depth analysis on their expressive power and relations to issues in MPNNs such as over-smoothing, over-squashing, and under-reaching.

3.1 EXPRESSIVE POWER

Intuitively, if the records of random walks contain enough information such that the structures of interest, e.g. graph G or local ball $B_r(v)$, can be fully recovered, a powerful reader NN such as an MLP (Hornik et al., 1989) or a transformer (Yun et al., 2020) on these records would be able to approximate any function of interest. Our analysis formalizes this intuition.

We first consider using an RWNN $X_\theta(\cdot)$ to universally approximate graph-level functions $\phi(\cdot)$ in probability, as defined in Abboud et al. (2021).

Definition 3.1. *$X_\theta(\cdot)$ is a universal approximator of graph-level functions in probability if, for all invariant functions $\phi : \mathbb{G}_n \to \mathbb{R}$ for a given $n \geq 1$, and $\forall \epsilon, \delta > 0$, there exist choices of length l of the random walk and network parameters θ such that the following holds:*

$$\mathrm{Prob}[|\phi(G) - X_\theta(G)| < \epsilon] > 1 - \delta, \quad \forall G \in \mathbb{G}_n. \tag{10}$$

We show that, if the random walk is long enough and the reader NN f_θ is universal, an RWNN $X_\theta(\cdot)$ is capable of graph-level universal approximation. The length of the walk l controls the confidence $> 1 - \delta$, with edge cover time $C_E(G)$ or vertex cover time $C_V(G)$ playing a central role.

[3]This is assuming that the random walks are localized in $B_r(v)$ and $B_r(u)$, e.g. with restarts.

Theorem 3.2. *An RWNN $X_\theta(\cdot)$ with a sufficiently powerful f_θ is a universal approximator of graph-level functions in probability (Definition 3.1) if it satisfies either of the below:*

- *It uses anonymization to record random walks of lengths $l > C_E(G)/\delta$.*
- *It uses anonymization + named neighbors to record walks of lengths $l > C_V(G)/\delta$.*

While both cover times are $O(n^3)$ for uniform random walks (Aleliunas et al., 1979; Zuckerman, 1991), we can use MDLR in Equation 6 to achieve an $O(n^2)$ vertex cover time, in conjunction with named neighborhood recording. While universality can be in principle achieved with uniform random walks, our design reduces the worst-case length l required for the desired reliability $> 1 - \delta$.

We now show an analogous result for universal approximation of vertex-level functions.

Definition 3.3. *$X_\theta(\cdot)$ is a universal approximator of vertex-level functions in probability if, for all invariant functions $\phi : \mathbb{B}_r \to \mathbb{R}$ for a given $r \geq 1$, and $\forall \epsilon, \delta > 0$, there exist choices of length l and restart probability α or period k of the random walk and network parameters θ such that:*

$$\text{Prob}[|\phi(B_r(v)) - X_\theta(G, v)| < \epsilon] > 1 - \delta, \quad \forall B_r(v) \in \mathbb{B}_r. \tag{11}$$

We show the following, using local vertex cover time $C_V(B_r(v))$ and edge cover time $C_E(B_r(v))$:

Theorem 3.4. *An RWNN $X_\theta(\cdot)$ with a sufficiently powerful f_θ and any nonzero restart probability α or restart period $k \geq r + 1$ is a universal approximator of vertex-level functions in probability (Definition 3.3) if it satisfies either of the below for all $B_r(v) \in \mathbb{B}_r$:*

- *It uses anonymization to record random walks of lengths $l > C_E(B_r(v))/\delta$.*
- *It uses anonymization + named neighbors to record walks of lengths $l > C_V(B_r(v))/\delta$.*

Since restarts are required to finitely bound the local cover times on an infinite graph (Section 2.2), non-restarting walks cannot support vertex-level universality in general, and our design is obligatory.

3.2 Over-smoothing, Over-squashing, and Under-reaching

Often, in MPNNs, each layer operates by passing features over edges and mixing them using weights deduced from e.g. adjacency matrix. This ties them to the topology of the input graph, and a range of prior work has shown how this relates to the well-known issues of over-smoothing, over-squashing, and under-reaching. We connect these results and RWNNs to verify if similar issues may take place.

Let G be a connected non-bipartite graph with row-normalized adjacency matrix P. We consider a linearized MPNN, where the vertex features $\mathbf{h}^{(0)}$ are initialized as some probability vector $\mathbf{x}$, and updated by $\mathbf{h}^{(t+1)} = \mathbf{h}^{(t)}P$. This simplification is often useful in understanding the aforementioned issues (Giraldo et al., 2023; Zhao & Akoglu, 2019). Specifically, in this model:

- Over-smoothing happens as the features exponentially converge to a stationary vector $\mathbf{h}^{(l)} \to \boldsymbol{\pi}$ as $l \to \infty$, smoothing out the input $\mathbf{x}$ (Giraldo et al., 2023).
- Over-squashing and under-reaching occur when a feature $\mathbf{h}_u^{(l)}$ becomes insensitive to distant input $\mathbf{x}_v$. While under-reaching refers to insufficient depth $l < \text{diam}(G)$ (Barceló et al., 2020), over-squashing refers to features getting overly compressed at bottlenecks of G, even with sufficient depth l. The latter is described by the Jacobian $|\partial \mathbf{h}_u^{(l)} / \partial \mathbf{x}_v| \leq [\sum_{t=0}^{l} P^t]_{uv}$,[4] as the bound often decays exponentially with l (Topping et al., 2022; Black et al., 2023).

What do these results tell us about RWNNs? We can see that, while P drives feature mixing in the message passing schema, it can be also interpreted as the transition probability matrix of uniform random walk where P_{uv} is the probability of walking from u to v. This parallelism motivates us to design an analogous, simplified RWNN and study its behavior.

We consider a simple RWNN that runs a uniform random walk $v_0 \to \cdots \to v_l$, reads the record $\mathbf{x}_{v_0} \to \cdots \to \mathbf{x}_{v_l}$ by averaging, and outputs it as $\mathbf{h}^{(l)}$. Like linear MPNN, the model involves l steps

[4] This bound is obtained by applying Lemma 3.2 of Black et al. (2023) to our linearized MPNN.

of time evolution through P. However, while MPNN uses P to process features, this model uses P only to obtain a record of input, with feature processing decoupled. We show that in this model, over-smoothing does not occur as in simple MPNNs[5]:

Theorem 3.5. *The simple RWNN outputs* $\mathbf{h}^{(l)} \to \mathbf{x}^\top \boldsymbol{\pi}$ *as* $l \to \infty$.

Even if the time evolution through P happens fast (i.e. P is rapidly mixing) or with many steps l, the model is resistant to over-smoothing as the input $\mathbf{x}$ always affects the output. In fact, if P is rapidly mixing, we may expect improved behaviors based on Section 3.1 as the cover times could reduce.

On the other hand, we show that over-squashing manifests as probabilistic under-reaching:

Theorem 3.6. *Let* $\mathbf{h}_u^{(l)}$ *be output of the simple RWNN queried with* u. *Then:*

$$\mathbb{E}\left[\left|\frac{\partial \mathbf{h}_u^{(l)}}{\partial \mathbf{x}_v}\right|\right] = \frac{1}{l+1}\left[\sum_{t=0}^{l} P^t\right]_{uv} \to \boldsymbol{\pi}_v \quad \textit{as} \quad l \to \infty. \tag{12}$$

The equation shows that the feature Jacobians are bounded by the sum of powers of P, same as in simple MPNN. Both models are subject to over-squashing phenomenon that is similarly formalized, but manifests through different mechanisms. While in message passing the term is related to over-compression of features at bottlenecks (Topping et al., 2022), in RWNNs it is related to exponentially decaying probability of reaching a distant vertex v, i.e. probabilistic under-reaching.

In many MPNNs, it is understood that the topology of the input graph inevitably induces a trade-off between over-smoothing and over-squashing (Nguyen et al., 2023; Giraldo et al., 2023). Our results suggest that RWNNs avoid the trade-off, and we can focus on overcoming under-reaching e.g. with long or rapidly-mixing walks, while not worrying much about over-smoothing. Design choices such as MDLR (Equation 6) and non-backtracking (Alon et al., 2007) can be understood as achieving this.

4 Related Work

We briefly review the related work. An extended discussion can be found in Appendix A.6.

Random walks for learning on graphs In graph learning, random walks have received interest due to compatibility with sequence learning methods (Table 1). DeepWalk (Perozzi et al., 2014) and node2vec (Grover & Leskovec, 2016) used skip-gram models on walks. CRaWl (Tönshoff et al., 2023) used 1D CNN on sliding window-based walk records, with expressive power bounded by the window size. We discuss the relation between CRaWl and our approach in depth in Appendix A.6. AgentNet (Martinkus et al., 2023) learns agents that walk on a graph while recurrently updating their features. While optimizing the walk strategy, this may trade off speed as training requires recurrent roll-out of the network. Our method allows pairing simple and fast walkers, such as MDLR, with parallelizable networks such as transformers. WalkLM (Tan et al., 2023) proposed a fine-tuning method for language models on walks on text-attributed graphs. By utilizing anonymization, our approach is able to process graphs even if no text attribute is given. Lastly, a concurrent work (Wang & Cho, 2024) arrived at a similar use of anonymization combined with RNNs.

Probabilistic invariant neural networks Whenever a learning problem is compatible with symmetry, incorporating the associated invariance structure to the hypothesis class often leads to generalization benefit (Bronstein et al., 2021; Elesedy, 2022; 2023). This is also the case for probabilistic invariant NNs (Lyle et al., 2020; Bloem-Reddy & Teh, 2020), which includes our approach. Probabilistic invariant NNs have recently gained interest due to their potential of achieving higher expressive powers compared to deterministic counterparts (Cotta et al., 2023; Sieradzki et al., 2022). In graph learning, this is often achieved with stochastic symmetry breaking between vertices using randomized features (Loukas, 2020; Puny et al., 2020; Abboud et al., 2021; Kim et al., 2022), vertex orderings (Murphy et al., 2019; Kim et al., 2023), or dropout (Papp et al., 2021). Our approach can be understood as using random walk as a symmetry-breaking mechanism for probabilistic invariance, which provides an additional benefit of natural compatibility with sequence learning methods.

[5]While we show not forgetting $\mathbf{x}$ for brevity, we may extend to initial vertex v_0 using its anonymization as 1.

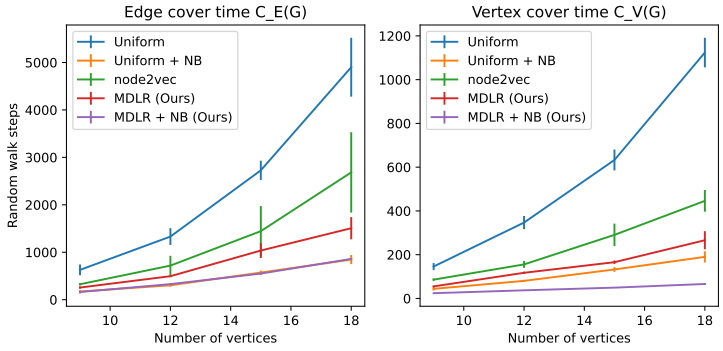

Figure 2: Cover times of random walks on varying sizes of lollipop graphs. NB is non-backtracking.

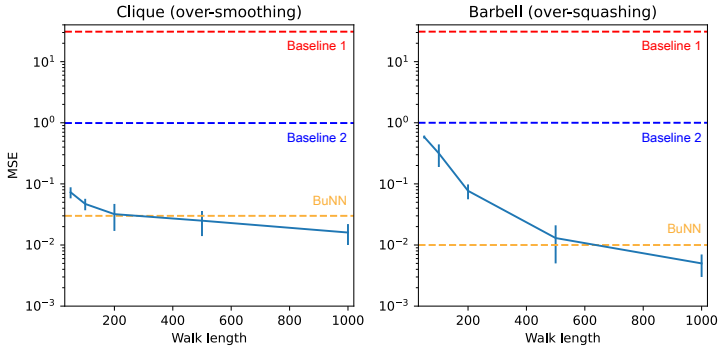

Figure 3: Over-smoothing and over-squashing (MSE ↓) for various walk lengths l.

Table 2: Over-smoothing and over-squashing results in comparison to baselines from Bamberger et al. (2024). We report aggregated mean squared error (MSE ↓) for 4 randomized runs.

Method	Clique (over-smoothing)	Barbell (over-squashing)
Baseline 1	30.94 ± 0.42	30.97 ± 0.42
Baseline 2	0.99 ± 0.08	1.00 ± 0.07
MLP	1.10 ± 0.08	1.08 ± 0.07
GCN	29.65 ± 0.34	1.05 ± 0.08
SAGE	0.86 ± 0.10	0.90 ± 0.29
GAT	20.97 ± 0.40	1.07 ± 0.09
NSD	0.08 ± 0.02	1.09 ± 0.15
BuNN	0.03 ± 0.01	0.01 ± 0.07
RWNN-transformer (Ours)	**0.016 ± 0.006**	**0.005 ± 0.002**

5 Experiments

We perform a series of experiments to demonstrate RWNNs. We implement random walk algorithms in C++ based on Chenebaux (2020), which produces good throughput (<0.1 seconds for 10k steps) even without GPU acceleration in (Tönshoff et al., 2023). Pseudocode is given in Appendix A.2. We implement our training and inference pipelines in PyTorch. Supplementary experiments including substructure counting, more real-world datasets, and link prediction, are in Appendix A.4.

5.1 Synthetic Experiments

On synthetic setups, we first verify our claims on cover times in Section 2.1, focusing on the utility of MDLR (Equation 6), non-backtracking, and neighborhood recording. We measure the edge cover times $C_E(G)$ and vertex cover times $C_V(G)$ of random walk algorithms discussed in the main text, on varying sizes of lollipop graphs G (Feige, 1995) which are commonly used to establish upper bounds of cover times. The results are in Figure 2. We find that **(1)** MDLR achieves a significant speed-up compared to uniform and node2vec walks, **(2)** adding non-backtracking significantly improves the behavior of base first-order walks in all cases, and **(3)** edge cover times are often much larger compared to vertex cover times, strongly justifying the use of neighborhood recording (Theorem 3.2).

Table 3: Isomorphism learning results. We report accuracy of classifying training data rounded to the first decimal point. *, †, ‡, §, and ⋄ are from Papp et al. (2021), Murphy et al. (2019), Zhao et al. (2022b), Martinkus et al. (2023), and Alvarez-Gonzalez et al. (2024), respectively.

Method	CSL 1, 2-WL fails	SR16 3-WL fails	SR25 3-WL fails
GIN	10.0%†	50.0%§	6.7%‡
PPGN	100.0%§	50.0%§	6.7%‡
GIN-AK+	-	-	6.7%‡
PPGN-AK+	-	-	100.0%‡
GIN+ELENE	-	-	6.7%⋄
GIN+ELENE-L (ED)	-	-	100.0%⋄
GIN-RNI	16.0%*	-	-
GIN-RP	37.6%†	-	-
GIN-Dropout	82.0%*	-	-
RW-AgentNet	100.0%§	50.5%§	-
AgentNet	100.0%§	100.0%§	6.7%
CRaWl	100.0%§	100.0%§	46.6%
RWNN-DeBERTa (Ours)	100.0%	100.0%	100.0%

Then, we verify our claims in Section 3.2 using Clique and Barbell datasets of Bamberger et al. (2024) that explicitly test for over-smoothing and over-squashing, respectively. Our RWNN uses MDLR walks with non-backtracking, and the reader NN is a 1-layer transformer encoder with width 128, matching the baselines. We precisely follow the experimental procedure of Bamberger et al. (2024). Figure 3 shows the results for varying walk lengths l. The model performs well on Clique overall, while Barbell requires scaling the walk length. This agrees with our claims in Section 3.2 that RWNNs in general avoid over-smoothing, but over-squashing manifests as probabilistic under-reaching (and is therefore mitigated by sufficiently long walks). With $l = 1000$, our model in Table 2 outperforms all baselines including BuNN which is specialized for mitigating over-smoothing and over-squashing.

5.2 Graph Isomorphism Learning

We now test the claims on expressive power in Section 3.1 using three challenging datasets where the task is recognizing the isomorphism type of input graph where certain WL test fails.

The Circular Skip Links (CSL) graphs dataset (Murphy et al., 2019) contains 10 non-isomorphic regular graphs with 41 vertices of degree 4. Distinguishing these graphs requires computing lengths of skip links, and 1-WL and 2-WL tests fail. The 4×4 rook's and Shrikhande graphs (Alvarez-Gonzalez et al., 2024), which we call SR16, are a pair of strongly regular graphs with 16 vertices of degree 6. Distinguishing the pair requires detecting 4-cliques, and 3-WL test fails. The SR25 dataset (Balcilar et al., 2021) contains 15 strongly regular graphs with 25 vertices of degree 12, on which 3-WL test fails. Examples of the considered graphs and random walks on them can be found in Appendix A.2.

Our RWNN uses MDLR random walk with non-backtracking, and recording function with anonymization and named neighbors that produces plain text (Algorithm 3). We use pre-trained DeBERTa-base language model as the reader NN to leverage its capacity, and fine-tune it with cross-entropy loss for at most 100k steps using AdamW optimizer with 2e-5 learning rate and 0.01 weight decay on 8× RTX 3090 GPUs. We truncate the input to 512 tokens which is the maximum allowed by memory constraint. We use batch size 256, and accumulate gradients for 8 steps for SR25. At test time, we ensemble 4 predictions of the network by averaging classification logits.

The results are in Table 3. MPNNs that align with certain WL test fail when asked to solve harder problems, e.g. GIN aligns with 1-WL and fails in CSL. A limited set of state-of-the art neural networks solve SR25, but at the cost of introducing specialized structural features (Alvarez-Gonzalez et al., 2024). Alternative approaches based on stochastic symmetry-breaking e.g. random node identification, often fail on CSL although universal approximation is possible in theory (Abboud et al., 2021), possibly due to learning difficulties. For algorithms based on walks, AgentNet and CRaWl solve CSL and SR16, while failing on SR25. This is because learning a policy to walk in AgentNet can be challenging in complex tasks especially at the early stage of training, and the expressiveness of CRaWl is limited by the receptive field of the 1D CNN. Our approach based on DeBERTa language model overcomes the problems, demonstrating as the first RWNN that solves SR25.

In Appendix A.3, we further provide visualizations of learned attentions by mapping attention weights on text records of walks to input graphs. We find that the models often focus on sparse, connected substructures, which presumably provide discriminative information on the isomorphism types.

Table 4: Test accuracy on ogbn-arxiv. † denotes using validation labels for label propagation or in-context learning following Huang et al. (2020). For Llama 3, we ensemble 5 predictions by voting.

Method	Accuracy
MLP	55.50%
node2vec	70.07%
GCN	71.74%
GraphSAGE	71.49%
GAT	73.91%
RevGAT	74.26%
Label propagation	68.50%
C&S	72.62%
C&S†	74.02%
Llama2-13b zero-shot	44.23%
GPT-3.5 zero-shot	73.50%
DeBERTa, fine-tuned	74.13%
Llama3-8b zero-shot	50.20%
Llama3-8b one-shot	52.49%
Llama3-8b one-shot†	52.54%
Llama3-70b zero-shot	65.33%
Llama3-70b one-shot†	67.57%
RWNN-Llama3-8b (Ours)	71.10%
RWNN-Llama3-8b (Ours)†	73.11%
RWNN-Llama3-70b (Ours)†	**74.75%**

5.3 Real-World Transductive Classification

Previous results considered tasks on undirected, unattributed, and relatively small graphs. We now show a preliminary result that RWNN based on Llama 3 (meta llama, 2024) language models can solve real-world problem on a large graph with directed edges and textual attributes. We use ogbn-arxiv (Hu et al., 2020), a citation network of 169,343 arXiv papers with title and abstract attributes. The task is transductive classification into 40 areas such as `"cs.AI"` using a set of labeled vertices.

We consider two representative types of baselines. The first reads title and abstract of each vertex using a language model and solves vertex-wise classification problem, ignoring graph structure. The second initializes vertex features as language model embeddings and trains an MPNN, at the risk of over-compressing the text. To take the best of both worlds, we design the recording function so that, not only it does basic operations such as anonymization, it records a complete information of the local subgraph including title and abstract, edge directions, and notably, **labels in case of labeled vertices** (Appendix A.2) (Sato, 2024). The resulting record naturally includes a number of input-label pairs of the classification task at hand, implying that we can frame transductive classification problem as a simple in-context learning problem (Brown et al., 2020). This allows training-free application of Llama 3 (meta llama, 2024) language model for transductive classification.

The results are in Table 4. Our models based on frozen Llama 3 perform competitively against a range of previous MPNNs on text embeddings, as well as outperforming language models that perform vertex-wise predictions ignoring graph structures such as GPT-3.5 and fine-tuned DeBERTa. Especially, our model largely outperforms one-shot baselines, which are given 40 randomly chosen labeled examples (one per class). This is surprising as our model observes fewer vertices, 29.17 in average, due to other recorded information. This is presumably since the record produced by our algorithm informs useful graph structure to the language model to quickly learn the task in-context compared to randomly chosen shots. In Appendix A.3, we visualize the attention weights, verifying that the model makes use of the graph structure recorded by random walks to make predictions.

As a final note, our approach is related to label propagation algorithms (Zhu & Ghahramani, 2002; Zhu, 2005; Grady, 2006) for transductive classification, which makes predictions by running random walks and probing the distribution of visited labeled vertices. The difference is, in our approach, the reader NN i.e. language model can appropriately use other information such as attributes, as well as do meaningful non-linear processing rather than simply probing the input. As shown in Table 4, our approach outperforms label propagation, verifying our intuition.

6 Conclusion

We contributed a principled understanding of RWNNs, where random walks on graphs are recorded and processed by NNs to make predictions. We analyzed invariance, expressive power, and information propagation, showing that we can design RWNNs to be invariant and universal without constraining its neural network. Experiments support the utility of our approach.

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A Appendix

A.1 Second-Order Random Walks (Section 2)

In second-order random walks, the probability of choosing v_{t+1} depends not only on v_t but also on v_{t-1}. We consider non-backtracking (Alon et al., 2007; Fitzner & van der Hofstad, 2013) and node2vec (Grover & Leskovec, 2016) random walks as representatives.

A non-backtracking random walk is defined upon a first-order random walk algorithm, e.g. one in Equation 4, by enforcing $v_{t+1} \neq v_{t-1}$:

$$\mathrm{Prob}[v_{t+1} = x | v_t = j, v_{t-1} = i] \coloneqq \begin{cases} \dfrac{\mathrm{Prob}[v_{t+1} = x | v_t = j]}{\sum_{y \in N(j) \setminus \{i\}} \mathrm{Prob}[v_{t+1} = y | v_t = j]} & \text{for } x \neq i, \\ 0 & \text{for } x = i, \end{cases} \tag{13}$$

where $\mathrm{Prob}[v_{t+1} = x | v_t = j]$ is the probability of walking $j \to x$ given by the underlying first-order random walk. Notice that the probabilities are renormalized over $N(j) \setminus \{i\}$. This is ill-defined in the case the walk traverses $i \to j$ and reaches a dangling vertex j which has i as its only neighbor, since $N(j) \setminus \{i\} = \emptyset$. In such cases, we allow the random walk to "begrudgingly" backtrack (Rappaport et al., 2017), $i \to j$ and then $j \to i$, given that it is the only possible choice due to the dangling of j.

In case of node2vec random walk (Grover & Leskovec, 2016), a weighting term $\alpha(v_{t-1}, v_{t+1})$ with two (hyper)parameters, return p and in-out q, is introduced to modify the behavior of a first-order random walk:

$$\mathrm{Prob}[v_{t+1} = x | v_t = j, v_{t-1} = i] \coloneqq \frac{\alpha(i, x) \, \mathrm{Prob}[v_{t+1} = x | v_t = j]}{\sum_{y \in N(j)} \alpha(i, y) \, \mathrm{Prob}[v_{t+1} = y | v_t = j]}, \tag{14}$$

where the probability $\mathrm{Prob}[v_{t+1} = x | v_t = j]$ is given by the underlying first-order random walk and $\alpha(v_{t-1}, v_{t+1})$ is defined as follows using the shortest path distance $d(v_{t-1}, v_{t+1})$:

$$\alpha(v_{t-1}, v_{t+1}) \coloneqq \begin{cases} 1/p & \text{for } d(v_{t-1}, v_{t+1}) = 0, \\ 1 & \text{for } d(v_{t-1}, v_{t+1}) = 1, \\ 1/q & \text{for } d(v_{t-1}, v_{t+1}) = 2. \end{cases} \tag{15}$$

Choosing a large return parameter p reduces backtracking since it decreases the probability of walking from v_t to v_{t-1}. Choosing a small in-out parameter q has a similar effect of avoiding v_{t-1}, with a slight difference that it avoids the neighbors of v_{t-1} as well.

We now show an extension of Proposition 2.2 to the above second-order random walks:

Proposition A.1. *The non-backtracking random walk in Equation 13 and the node2vec random walk in Equation 14 are invariant if their underlying first-order random walk algorithm is invariant.*

Proof. The proof is given in Appendix A.5.3. □

A.2 Main Algorithm

We outline the main algorithms for the random walk and the recording function described in Section 2 and used in Section 5. Algorithm 1 shows the random walk algorithm, and Algorithms 2, 3, and 4 show the recording functions. For the random walk algorithm, we use non-backtracking described in Appendix A.1 and the minimum degree local rule conductance $c_G(\cdot)$ given in Equation 6 by default.

Based on the algorithms, in Figures 4, 5, and 6 we illustrate the task formats used for graph separation experiments in Section 5.2 by providing examples of input graphs, text records of random walks on them, and prediction targets for the language model that processes the records. Likewise, in Figures 7, 8, and 9 we show task formats for transductive classification on arXiv citation network in Section 5.3.

Algorithm 1: Random walk algorithm

Data: Input graph G, optional input vertex v, conductance function $c_G : E(G) \to \mathbb{R}_+$, walk length l, optional restart probability $\alpha \in (0, 1)$ or period $k > 1$
Result: Random walk $v_0 \to \cdots \to v_l$, restart flags $r_1, ..., r_l$

```
/* transition probabilities p : E(G) → ℝ+ */
for (u, x) ∈ E(G) do
    p(u, x) ← c_G(u, x) / Σ_{y∈N(u)} c_G(u, y)                    // Equation 4
/* starting vertex v_0 */
if v is given then
    /* query starting vertex */
    v_0 ← v
else
    /* sample starting vertex */
    v_0 ~ Uniform(V(G))
/* random walk v_1 → ··· → v_l, restart flags r_1, ..., r_l */
v_1 ~ Categorical({p(v_0, x) : x ∈ N(v_0)})
r_1 ← 0
for t ← 2 to l do
    /* restart flag r_t */
    r_t ← 0
    if α is given then
        /* if restarted at t − 1, do not restart */
        if r_{t−1} = 0 then
            r_t ~ Bernoulli(α)
    else if k is given then
        if t ≡ 0 (mod k) then
            r_t ← 1
    /* random walk v_t */
    if r_t = 0 then
        S ← N(v_{t−1}) \ {v_{t−2}}
        if S ≠ ∅ then
            /* non-backtracking */
            v_t ~ Categorical({p(v_{t−1}, x) / Σ_{y∈S} p(v_{t−1}, y) : x ∈ S})    // Equation 13
        else
            /* begrudgingly backtracking */
            v_t ← v_{t−2}
    else
        /* restart */
        v_t ← v_0
```

Algorithm 2: Recording function, using anonymization

Data: Random walk $v_0 \to \cdots \to v_l$, restart flags $r_1, ..., r_l$
Result: Text record $\mathbf{z}$

```
/* named vertices S, namespace id(·) */
S ← {v_0}
id(v_0) ← 1
/* text record z */
z ← id(v_0)
for t ← 1 to l do
    /* anonymization v_t ↦ id(v_t) */
    if v_t ∉ S then
        S ← S ∪ {v_t}
        id(v_t) ← |S|
    /* text record z */
    if r_t = 0 then
        /* record walk v_{t-1} → v_t */
        z ← z + "-" + id(v_t)
    else
        /* record restart v_t = v_0 */
        z ← z + ";" + id(v_t)
```

Algorithm 3: Recording function, using anonymization and named neighbors

Data: Random walk $v_0 \to \cdots \to v_l$, restart flags $r_1, ..., r_l$, input graph G
Result: Text record $\mathbf{z}$

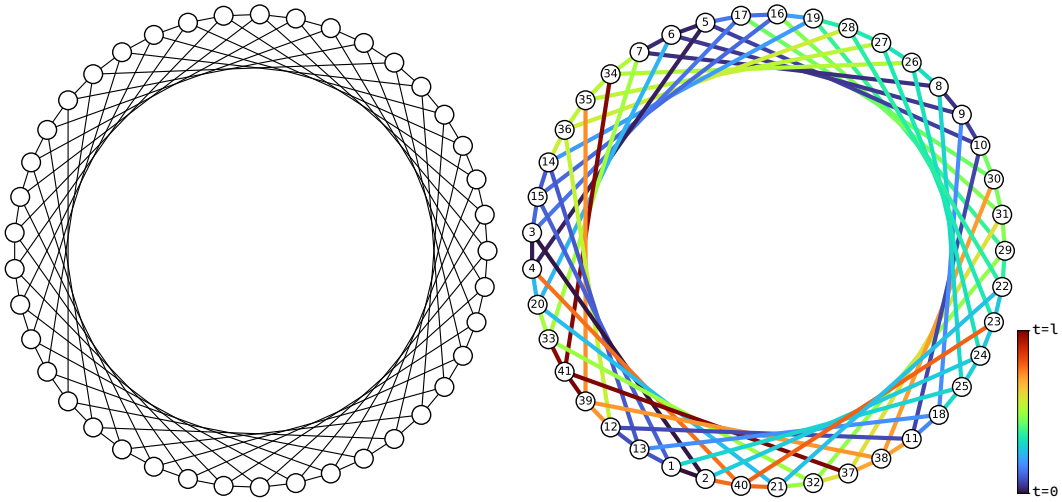
```
/* named vertices S, namespace id(·), recorded edges T */
S ← {v_0}
id(v_0) ← 1
T ← ∅
/* text record z */
z ← id(v_0)
for t ← 1 to l do
    /* anonymization v_t ↦ id(v_t) */
    if v_t ∉ S then
        S ← S ∪ {v_t}
        id(v_t) ← |S|
    /* text record z */
    if r_t = 0 then
        /* record walk v_{t-1} → v_t */
        z ← z + "-" + id(v_t)
        T ← T ∪ {(v_{t-1}, v_t), (v_t, v_{t-1})}
        /* named neighborhood U */
        U ← N(v_t) ∩ S
        if U ≠ ∅ then
            /* sort in ascending order id(u_1) < ··· < id(u_{|U|}) */
            [u_1, ..., u_{|U|}] ← SortByKey(U, id)
            for u ← u_1 to u_{|U|} do
                /* record named neighbors v_t → u */
                if (v_t, u) ∉ T then
                    z ← z + "#" + id(u)
                    T ← T ∪ {(v_t, u), (u, v_t)}
    else
        /* record restart v_t = v_0 */
        z ← z + ";" + id(v_t)
```

Algorithm 4: Recording function for transductive classification on arXiv network (Section 5.3)

Data: Directed input graph G, random walk $v_0 \to \cdots \to v_l$ and restart flags $r_1, ..., r_l$ on the undirected copy of G, paper titles $\{\mathbf{t}_v\}_{v \in V(G)}$ and abstracts $\{\mathbf{a}_v\}_{v \in V(G)}$, target category labels $\{\mathbf{y}_v\}_{v \in L}$ for labeled vertices $L \subset V(G)$

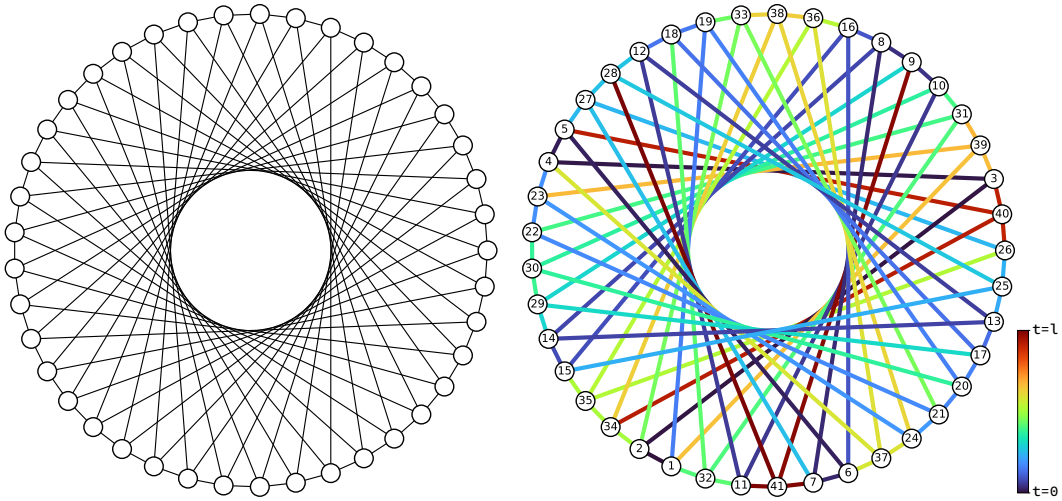
Result: Text record $\mathbf{z}$

```
/* named vertices S, namespace id(·), recorded edges T */
S ← {v_0}
id(v_0) ← 1
T ← ∅
/* text record z */
/* record starting vertex */
z ← "Paper 1 - Title: {t_{v_0}}", Abstract: {a_{v_0}}"
for t ← 1 to l do
    /* anonymization v_t ↦ id(v_t) */
    if v_t ∉ S then
        S ← S ∪ {v_t}
        id(v_t) ← |S|
    /* text record z */
    if r_t = 0 then
        /* record walk v_{t-1} → v_t with direction */
        if (v_{t-1}, v_t) ∈ E(G) then
            z ← z + " Paper {id(v_{t-1})} cites Paper {id(v_t)}"
        else
            z ← z + " Paper {id(v_{t-1})} is cited by Paper {id(v_t)}"
        T ← T ∪ {(v_{t-1}, v_t), (v_t, v_{t-1})}
        /* record title t_v, abstract a_v, and label y_v if v is labeled */
        if id(v_t) = |S| then
            z ← z + " - {t_v}"
            if v ∈ L then
                z ← z + ", Category: {y_v}"
            z ← z + ", Abstract: {a_v}"
        else
            z ← z + "."
        /* named neighborhood U */
        U ← N(v_t) ∩ S
        if U ≠ ∅ then
            /* sort in ascending order id(u_1) < ··· < id(u_{|U|}) */
            [u_1, ..., u_{|U|}] ← SortByKey(U, id)
            for u ← u_1 to u_{|U|} do
                /* record named neighbors v_t → u with directions */
                if (v_t, u) ∉ T then
                    if (v_t, u) ∈ E(G) then
                        z ← z + " Paper {id(v_t)} cites Paper {id(u)}."
                    else
                        z ← z + " Paper {id(v_t)} is cited by Paper {id(u)}."
                    T ← T ∪ {(v_t, u), (u, v_t)}
    else
        /* record restart */
        z ← z + " Restart at Paper 1."
```



Graph | Random Walk

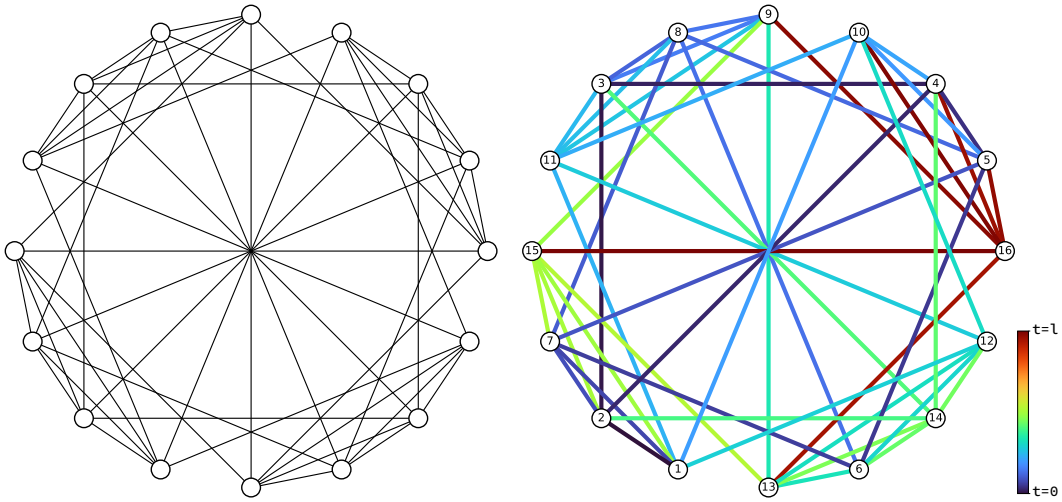
Record	[CLS]1-2-3-4-5-6-7-8-9#6-10#5-11-12-13#1-14-15#1#3-16-17#3#5-5-10-11-18#9#13-13-14-19#16-16-17-5-6-20#4-21-22-23-24#2-25#1#8#18-8-26#24-27#23-28#19#22-22-29#19-19-14-13-18-11-10-5-17-30#10-31#16#29-29-32#21-33#7#20-7-34#26-35#27-36#12#14#28-28-22-29-31-37#32-32-33-7-6-5-4-20-6-5-4-20-33-32-37-38#11#30-39#12#35-12-11-10-5-4-40#2#21#23-2-24-23-27-28-19-16-17-30-10-5-4-40-2-3-4-5-17-3-2-40-4-20-33-32-21-20-33-41#34#37#39-39-38-37-31-29-32-33-41-34-35-36-28-27-35-39-12-13-1-15-3-4-20-6-7-33-41-34-35-39-41-37-32-33-20-21-40-23-22-29-31-37-41-34-35-39-12-13-18-25-24-26-34-7-33-20-4-40-23-27-35-36-12-11-10-30-31-16-15-3-4-40-23-22-28-36-14-19-29-31-37-41-33-32-29-22-21-32-33-20-4-40-21-22-29-19-14-15-16-31-29-[SEP]
Answer	csl(41, 9)



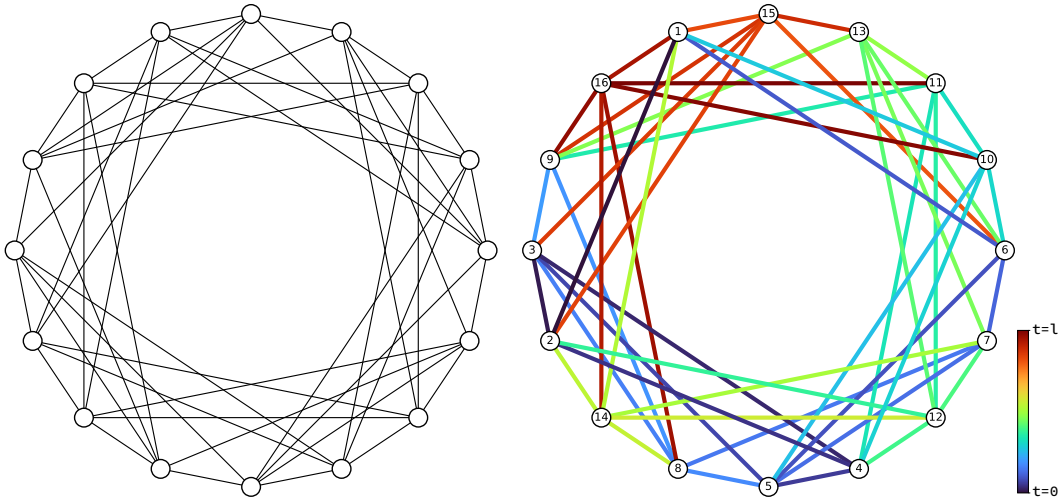
Graph | Random Walk

Record	[CLS]1-2-3-4-5-6-7-8-9-10-11-12-13-14#8-15-16#6#8-6-7-8-14-13-17-18#12-19#1-20#17-21-22-23#4-24#21-21-20-17-13-25#15-26-27#5#7-28#12#25-12-13-14-29#9#17-17-13-25-28-12-13-14-8-9-10-30#20#22#29-22-31#10-32#1#11#18-1-19-33#2#21-21-22-31-32-1-19-33-2-34-35#15#26-36#16-16-15-25-28-27-7-6-37#4#24#36-4-23-24-38#33#34#36-34-2-1-39#3#23#31-23-24-38-33-19-1-2-3-39-23-24-21-33-38-24-23-4-37-24-23-39-1-2-34-38-36-37-6-5-4-23-39-3-4-5-6-16-15-35-26-40#3#5#34-5-6-7-27-28-12-13-17-29-9-41#7#11#28-7-27-26-25-13-12-11-32-18-12-13-14-15-25-26-40-34-38-36-37-24-23-4-37-24-21-33-2-3-4-5-27-7-6-16-15-35-34-2-3-40-26-35-34-38-33-21-20-17-29-14-15-16-8-9-41-28-27-7-8-14-15-25-28-27-5-6-7-41-9-8-7-41-9-10-31-[SEP]
Answer	csl(41, 16)

Figure 4: Two CSL graphs and text records of random walks from Algorithms 1 and 3. Task is graph classification into 10 isomorphism types $\mathrm{csl}(41, s)$ for skip length $s \in \{2, 3, 4, 5, 6, 9, 11, 12, 13, 16\}$. In random walks, we label vertices by anonymization and color edges by their time of discovery.

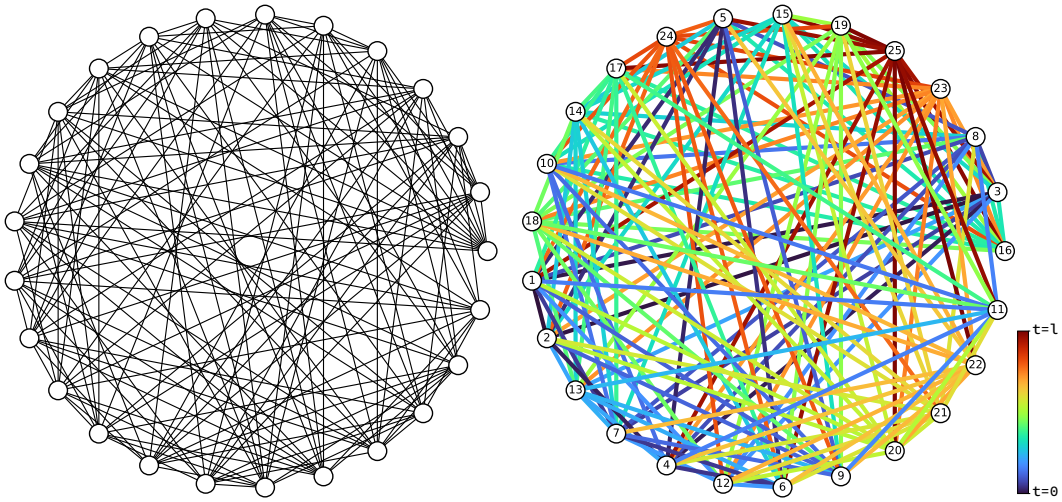


Record	[CLS]1-2-3-4#2-5-6-7#1#2#5-8#3#5#6-9#3-3-4-5-10#1#4-11#1#3#8#9-12#1#6#10-13#6#9-6-5-8-7-2-14#3#4#6#12#13-13-9-15#1#2#7#13-7-6-13-12-1-2-4-10-12-11-1-7-15-1-11-12-10-4-14-13-15-2-7-8-9-3-2-7-8-5-7-2-3-14-13-15-1-2-14-13-16#4#5#9#10#15-5-10-1-11-3-14-4-16-10-1-12-13-6-12-13-6-12-10-11-12-10-11-1-7-6-13-15-16-5-4-14-3-9-13-16-15-1-12-13-9-15-7-2-14-13-6-5-7-2-4-3-9-15-13-14-6-5-7-8-9-11-10-5-16-4-3-14-2-15-13-12-10-5-16-4-14-13-12-14-13-16-10-5-6-14-3-9-16-13-9-15-1-2-15-7-1-12-13-6-8-5-7-6-12-1-11-12-14-4-2-15-9-8-7-1-15-16-4-14-12-1-10-5-16-9-8-5-16-13-12-6-14-2-1-7-15-16-4-2-1-15-16-10-4-16-15-9-16-15-13-6-8-9-16-5-6-[SEP]
Answer	4×4 rook's graph

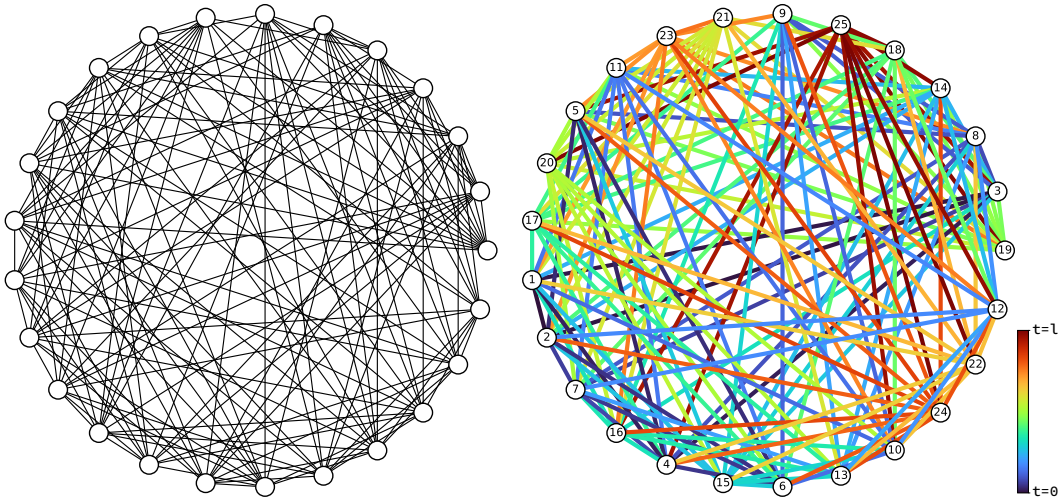


Record	[CLS]1-2-3-4#2-5#3-6#1-7#5-8#3#5-9#3-3-4-5-10#1#4#6-11#4#9-12#2#4#7-13#6#7#9#11-7-14#1#2#8#12-8-5-6-7-13-9-11-4-5-3-4-12-14-1-10-6-15#1#2#3#9#13-2-14-16#1#8#9#10#11-10-11-4-10-6-1-16-8-7-5-8-9-3-5-7-8-14-7-6-15-2-3-8-14-2-1-16-11-4-10-6-15-13-6-1-16-10-6-1-16-14-12-13-7-12-4-3-2-12-11-4-5-7-13-15-3-5-6-1-15-9-13-11-16-10-6-13-9-11-4-12-7-13-6-7-5-6-1-15-9-11-13-6-5-4-2-3-9-15-1-14-16-1-15-6-7-13-15-1-10-5-3-2-1-16-10-4-11-16-10-5-4-12-11-9-16-11-9-13-12-14-16-1-10-4-11-12-13-6-5-7-12-2-3-5-4-10-6-13-9-8-5-10-16-11-12-2-1-6-10-5-3-9-8-14-16-11-10-5-6-7-12-14-16-11-12-14-1-16-11-10-4-11-13-9-16-8-3-5-8-9-16-14-2-[SEP]
Answer	Shrikhande graph

Figure 5: SR16 graphs and text records of random walks from Algorithms 1 and 3. The task is graph classification into two isomorphism types $\{4 \times 4$ rook's graph, Shrikhande graph$\}$. In random walks, we label vertices by anonymization and color edges by their time of discovery.



Record	[CLS]1-2-3#1-4#2-5#1#2-6#4-7#1#3-3-8#1#4#5#7-5-9#1#2#7-10#4#7#8-11#1#4#8#9-8-12#1#3#6#7-3-13#2#4#6#7#9#11-2-3-7-6-14#2#5#7#8#13-15#2#3#7#9#10-16#3#5#8#10#14-17#1#6#7#10#11#13#14-13-18#5#8#9#11#12#14#16-19#3#6#9#11#12#13#15#16-9-7-13-11-20#1#2#12#14#15#17#18-21#2#4#6#8#10#11#12#14#15#19-8-7-14-5-22#4#6#7#9#10#12#15#18#20-23#2#3#4#10#12#13#16#17#18#20-13-9-2-21-24#1#2#5#6#9#10#12#16#17#19#23-19-6-24-23-16-3-1-5-8-21-14-2-3-7-8-5-6-7-1-25#3#4#5#6#11#15#16#17#19#20#22-17-1-11-4-3-15-20-2-5-22-12-21-14-7-9-5-4-22-20-25-11-21-8-1-24-17-10-23-18-13-6-4-8-3-7-17-14-20-12-24-16-17-10-21-14-5-4-13-14-7-13-3-8-1-3-7-14-13-2-3-8-18-22-5-[SEP]
Answer	Graph 1



Record	[CLS]1-2-3#1-4#1-5#2-6#2#4-7#2#3#4-3-8#4#5#7-9#3#6-10#1#6-11#1#4#6#7#8-12#2#7#8#10-8-13#7#9#12-14#1#2#3#11#12-15#1#2#3#5#6#8#9#10#13-1-3-16#1#4#7#9#10#13-13-17#1#4#6#9#11#14-18#2#3#6#7#9#10#12-19#3#5#8#9#11#14#17-11-7-20#5#6#10#11#13#14#15#16#19-21#1#2#5#7#13#16#17#18#19-16-13-15-22#1#4#5#8#10#12#13#17#18#21-10-6-18-7-11-23#1#2#5#8#9#10#12#16#19#21-12-8-4-24#2#5#6#9#12#13#14#16#17#23-16-10-23-9-6-5-8-19-3-1-23-8-22-5-2-3-16-25#3#4#5#10#12#14#18#19#20#22#24-14-13-16-1-21-17-1-22-15-3-9-13-16-21-22-15-10-11-4-24-9-6-10-12-14-24-12-8-7-11-20-5-25-20-7-6-4-8-3-16-21-20-13-15-5-19-23-5-6-17-9-6-7-11-4-7-3-8-7-3-16-23-2-1-3-8-5-24-23-[SEP]
Answer	Graph 8

Figure 6: Two SR25 graphs and text records of random walks from Algorithms 1 and 3. The task is graph classification into 15 isomorphism types. In random walks, we label vertices by anonymization and color edges by their time of discovery.

System	A walk on the arXiv citation network will be given. Predict the arXiv CS sub-category Paper 1 belongs to. It is one of the following: Numerical Analysis (cs.NA), Multimedia (cs.MM), Logic in Computer Science (cs.LO), ... Discrete Mathematics (cs.DM). Only respond with the answer, do not say any word or explain.
Record	A walk on arXiv citation network is as follows: Paper 1 - Title: Safety guided deep reinforcement learning via online gaussian process estimation, Abstract: An important facet of reinforcement learning (rl) has to do with how the agent goes about exploring the environment. traditional exploration strategies typically focus on efficiency and ignore safety. however, for practical applications, ensuring safety of the agent during exploration is crucial since performing an unsafe action or reaching an unsafe state could result in irreversible damage to the agent. the main challenge of safe exploration is that characterizing the unsafe states and actions... Restart at 1. Paper 1 is cited by 2 - Learning to walk in the real world with minimal human effort, Abstract: Reliable and stable locomotion has been one of the most fundamental challenges for legged robots. deep reinforcement learning (deep rl) has emerged as a promising method for developing such control policies... Restart at 1. Paper 1 cites 3 - Deep q learning from demonstrations, Category: Artificial Intelligence (cs.AI), Abstract: Deep reinforcement learning (rl) has achieved several high profile successes in difficult decision-making problems. however, these algorithms typically require a huge amount of data before they reach... Restart at 1. Paper 1 cites 4 - Constrained policy optimization, Category: Machine Learning (cs.LG), Abstract: For many applications of reinforcement learning it can be more convenient to specify both a reward function and constraints, rather than trying to design behavior through the reward function. for example,... Paper 4 is cited by 2. Paper 4 is cited by 5 - Artificial intelligence values and alignment, Abstract: This paper looks at philosophical questions that arise in the context of ai alignment. it defends three propositions. first, normative and technical aspects of the ai alignment problem are interrelated,... Paper 5 cites 6 - Agi safety literature review, Category: Artificial Intelligence (cs.AI), Abstract: The development of artificial general intelligence (agi) promises to be a major event. along with its many potential benefits, it also raises serious safety concerns (bostrom, 2014). the intention of... Paper 6 is cited by 7 - Modeling agi safety frameworks with causal influence diagrams, Abstract: Proposals for safe agi systems are typically made at the level of frameworks, specifying how the components of the proposed system should be trained and interact with each other. in this paper, we model... Restart at 1. Paper 1 cites 8 - Safe learning of regions of attraction for uncertain nonlinear systems with gaussian processes, Category: Systems and Control (cs.SY), Abstract: Control theory can provide useful insights into the properties of controlled, dynamic systems. one important property of nonlinear systems is the region of attraction (roa), a safe subset of the state... Paper 8 is cited by 9 - Control theory meets pomdps a hybrid systems approach, Abstract: Partially observable markov decision processes (pomdps) provide a modeling framework for a variety of sequential decision making under uncertainty scenarios in artificial intelligence (ai). since the... Restart at 1. ... Which arXiv CS sub-category does Paper 1 belong to? Only respond with the answer, do not say any word or explain.
Answer	Machine Learning (cs.LG)

Figure 7: Transductive classification on arXiv citation network using text record of random walk from Algorithms 1 and 4. Colors indicate task instruction, walk information, and label information.

System	Title and abstract of an arXiv paper will be given. Predict the arXiv CS sub-category the paper belongs to. It is one of the following: Numerical Analysis (cs.NA), Multimedia (cs.MM), Logic in Computer Science (cs.LO), ... Discrete Mathematics (cs.DM). Only respond with the answer, do not say any word or explain.
Context	Title: Safety guided deep reinforcement learning via online gaussian process estimation Abstract: An important facet of reinforcement learning (rl) has to do with how the agent goes about exploring the environment. traditional exploration strategies typically focus on efficiency and ignore safety. however, for practical applications, ensuring safety of the agent during exploration is crucial since performing an unsafe action or reaching an unsafe state could result in irreversible damage to the agent. the main challenge of safe exploration is that characterizing the unsafe states and actions... Which arXiv CS sub-category does this paper belong to?
Answer	Machine Learning (cs.LG)

Figure 8: Zero-shot format for vertex classification on arXiv citation network. Task instruction and label information are colored.

System	Title and abstract of an arXiv paper will be given. Predict the arXiv CS sub-category the paper belongs to. It is one of the following: Numerical Analysis (cs.NA), Multimedia (cs.MM), Logic in Computer Science (cs.LO), ... Discrete Mathematics (cs.DM).
Context	Title: Deeptrack learning discriminative feature representations online for robust visual tracking Abstract: Deep neural networks, albeit their great success on feature learning in various computer vision tasks, are usually considered as impractical for online visual tracking, because they require very long... Category: cs.CV Title: Perceived audiovisual quality modelling based on decison trees genetic programming and neural networks... Abstract: Our objective is to build machine learning based models that predict audiovisual quality directly from a set of correlated parameters that are extracted from a target quality dataset. we have used the... Category: cs.MM ... Title: Safety guided deep reinforcement learning via online gaussian process estimation Abstract: An important facet of reinforcement learning (rl) has to do with how the agent goes about exploring the environment. traditional exploration strategies typically focus on efficiency and ignore safety. however, for practical applications, ensuring safety of the agent during exploration is crucial since performing an unsafe action or reaching an unsafe state could result in irreversible damage to the agent. the main challenge of safe exploration is that characterizing the unsafe states and actions... Which arXiv CS sub-category does this paper belong to?
Answer	cs.LG

Figure 9: One-shot format for transductive classification on arXiv citation network. 40 labeled examples are given in form of multi-turn dialogue. Task instruction and label information are colored.

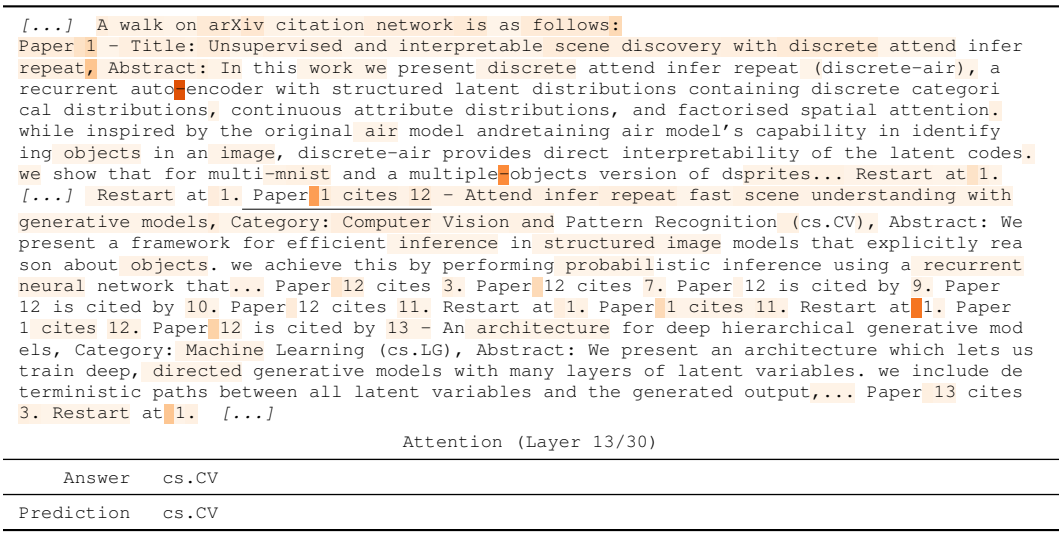


Figure 10: Example of attention in a frozen Llama 3 8B applied on arXiv transductive classification. Attention weights are averaged over all 30 heads.

A.3 Attention Visualizations

In Figure 10, we show an example of self-attention in the frozen Llama 3 8B model applied to arXiv transductive classification (Section 5.3). We show attention weights on text record of random walk from the generated `cs` token as query, which is just before finishing the prediction e.g. `cs.CV`. We color the strongest activation with orange, and do not color values below 1% of it. The model invests a nontrivial amount of attention on walk information such as `Paper 1 cites 12`, while also making use of titles and labels of labeled vertices. This indicates the model is utilizing the graph structure recorded by the random walk in conjunction with other information to make predictions.

In Figures 11, 12, and 13, we show examples of self-attention in DeBERTa models trained for graph separation (Section 5.2). We first show attention weights on text record of random walk from the `[CLS]` query token. Then, we show an alternative visualization where the attention weights are mapped onto the original input graph. For example, for each attention on v_{t+1} where the walk has traversed $v_t \to v_{t+1}$, we regard it as an attention on the edge (v_t, v_{t+1}) in the input graph. We ignore `[CLS]` and `[SEP]` tokens since they do not appear on the input graph. We observe that the models often focus on sparse, connected substructures, which presumably provide discriminative information on the isomorphism types. In particular, for CSL graphs (Figure 11) we observe an interpretable pattern of approximate cycles composed of skip links. This is presumably related to measuring the lengths of skip links, which provides sufficient information of isomorphism types of CSL graphs.

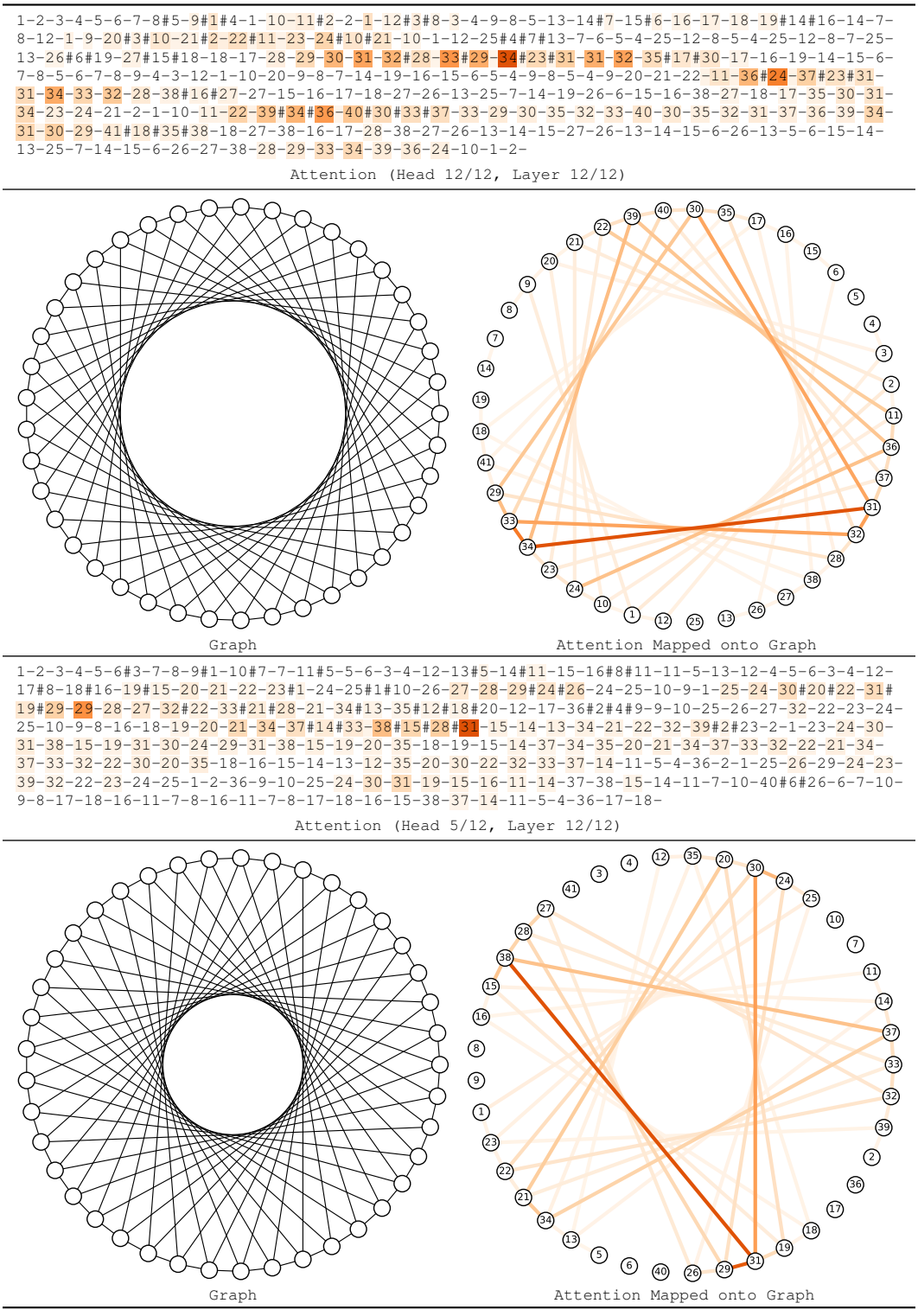


Figure 11: Examples of attention from [CLS] token in a DeBERTa trained on CSL graph separation, forming approximate cycles using skip links. This is presumably related to measuring the lengths of skip links, which provides sufficient information to infer isomorphism types of CSL graphs.

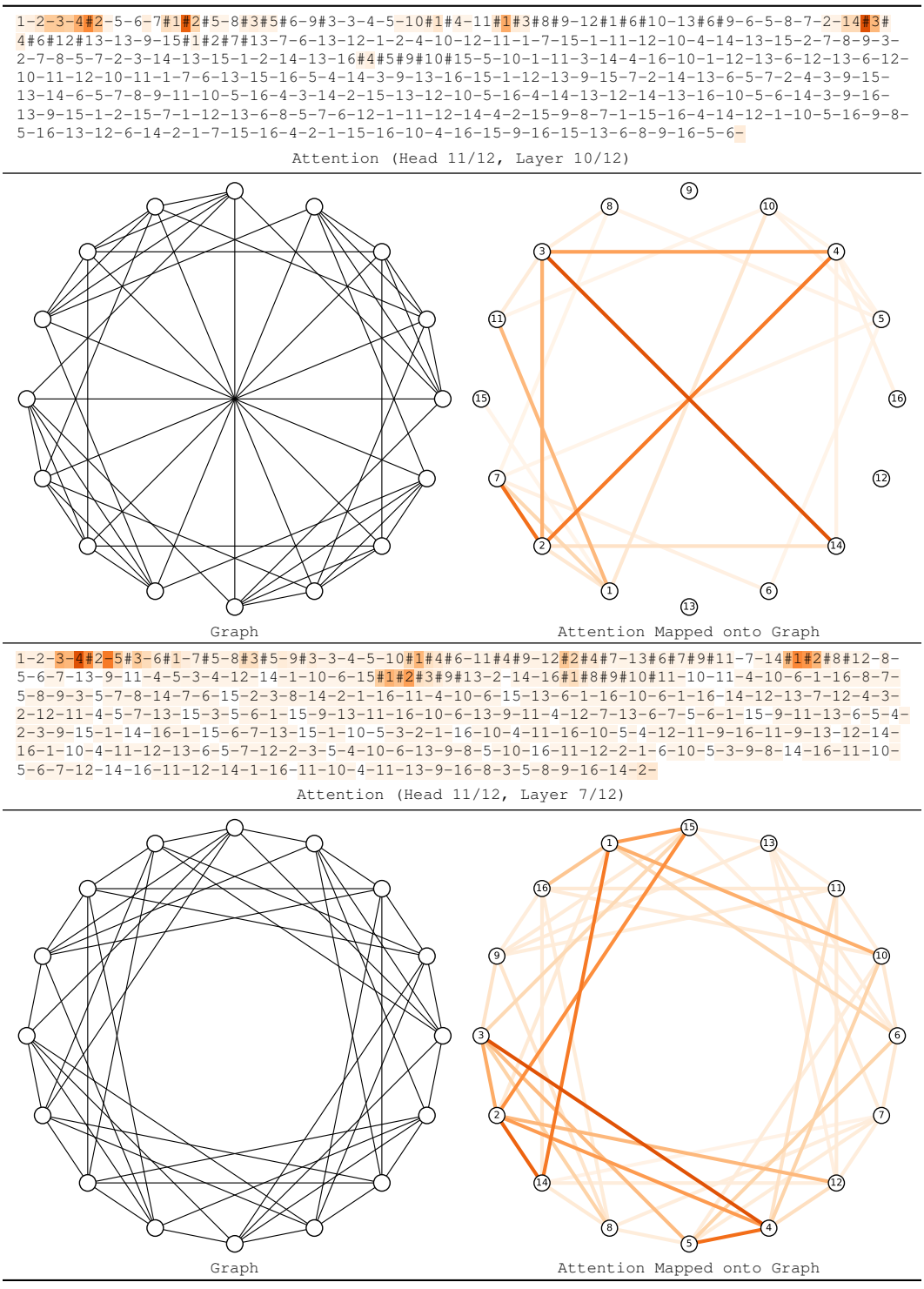


Figure 12: Examples of attention from [CLS] token in a DeBERTa trained on SR16 graph separation. The model tend to focus on neighborhood records that form a sparse connected substructure, which we conjecture to provide discriminative information on the isomorphism type of SR16 graphs.

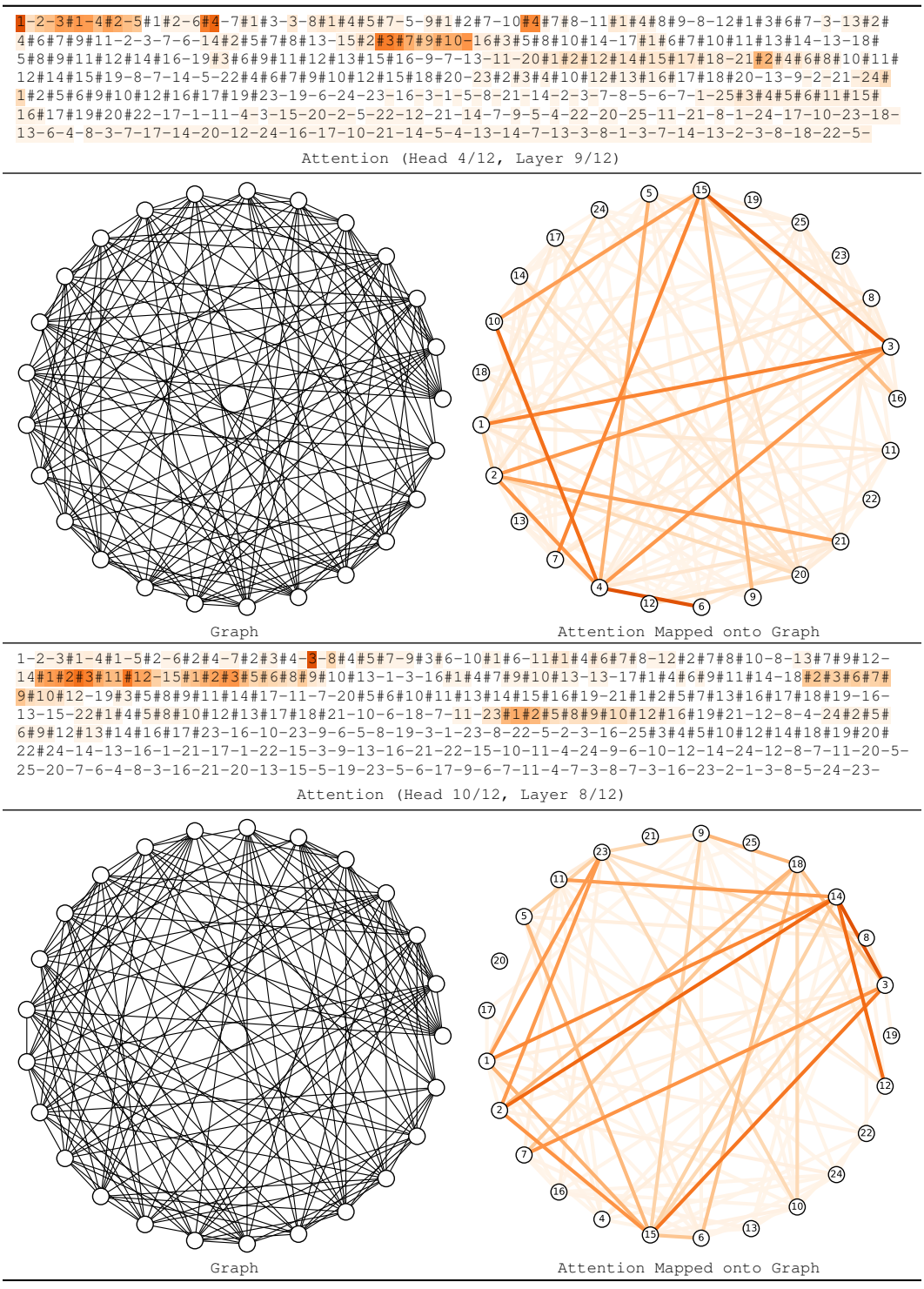


Figure 13: Examples of attention from [CLS] token in a DeBERTa trained on SR25 graph separation. The model tend to focus on neighborhood records that form a sparse connected substructure, which we conjecture to provide discriminative information on the isomorphism type of SR25 graphs.

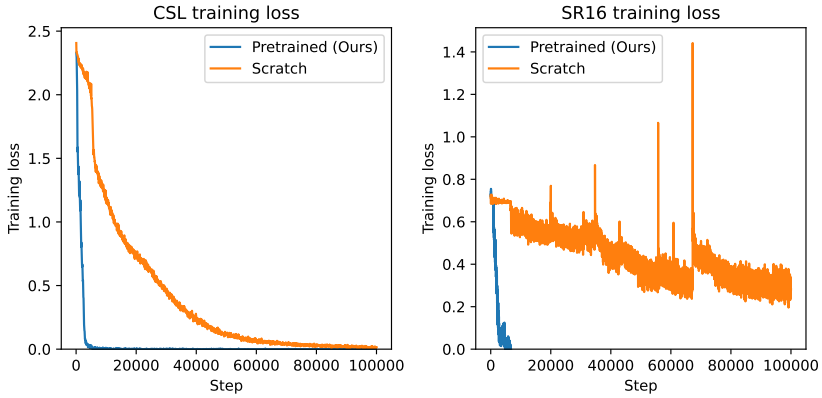


Figure 14: The impact of language pre-training for graph isomorphism learning (Section 5.2).

```
Record  1[O,sp2]=π2[C,d:3,sp2,r]-3[C,cw,d:4,H:1,sp3,r]-4[N,d:3,H:1,sp2,r]-
        π5[C,d:3,sp2,r]=π6[O,sp2]=π5-π4-3-2=π1=π2-3-7[C,d:4,H:2,sp3,r]-8[S,d:2,sp3,r]-
        9[S,d:2,sp3,r]-10[C,d:4,H:2,sp3,r]-11[C,ccw,d:4,H:1,sp3,r]-12[N,d:3,H:1,sp2,r]-
        π13[C,d:3,sp2,r]=π14[O,sp2]=π13-π12-11-15[C,d:3,sp2,r]-π16[N,d:3,H:1,sp2,r]-
        17[C,cw,d:4,H:1,sp3,r]-18[C,d:3,sp2,r]=π19[O,sp2]=π18-17-20[C,d:4,H:2,sp3]-
        21[C,d:4,H:2,sp3]-22[C,d:3,sp2]=π23[O,sp2]=π22-π24[O,d:2,H:1,sp2]-π22=π23=
        π22-π24-π22=π23=π22-21-20-17-16-π15=π25[O,sp2]=π15-π16-17-20-21-22-π24-π22=
        π23=π22-21-20-17-16-π15=π25=π15-π16-17-20-21-22-π24-π22=π23=π22-π24-π22-21-
        20-17-18=π19=π18-π26[N,d:3,H:1,sp2,r]-27[C,ccw,d:4,H:1,sp3,r]-28[C,d:3,sp2]=
        π29[O,sp2]=π28-π30[N,d:3,H:1,sp2]-31[C,ccw,d:4,H:1,sp3]-32[C,d:4,H:1,sp3]-
        33[C,d:4,H:3,sp3]-32-34[C,d:4,H:3,sp3]-32-33-32-34-32-33-32-34-32-33-32-31-30-
        π28=π29=π28-π30-31-32-34-32-31-30-π28=π29=π28-π30-31-32-33-32-34-32-33-32-34-
        32-31-30-π28=π29=π28-π30-31-35[C,d:3,sp2]=π36[O,sp2]=π35-π37[N,d:3,H:1,sp2]-
        38[C,cw,d:4,H:1,sp3]-39[C,d:3,sp2]-π40[N,d:3,H:1,sp2]-41[C,cw,d:4,H:1,sp3]-
        42[C,d:4,H:2,sp3]-43[C,d:3,sp2,*,r]*π44[C,d:3,H:1,sp2,*,r]*π45[N,d:3,H:1,sp2,*
        ,r]*π46[C,d:3,H:1,sp2,*,r]*π47[N,d:2,sp2,*,r]#*π43*π43*π44*π45*π46*π47*π43-42-41-
        40-π39=π48[O,sp2]=π39-38-37-π35=π36=π35-π37-38-49[C,d:4,H:2,sp3]-50[C
```

Figure 15: An example text record for Peptides-func graph classification.

Table 5: Peptides-func graph classification. The baseline scores are from Tönshoff et al. (2023).

Method	Test AP
GCN	0.5930
GINE	0.5498
GatedGCN	0.6069
Transformer	0.6326
SAN	0.6439
CRaWl	0.7074
RWNN-DeBERTa (Ours)	**0.7124 ± 0.0016**

A.4 Supplementary Experiments

We include supplementary experiments we could not include in the main text due to space constraints.

A.4.1 The Benefit of Language Pre-training (Section 5.2)

In Section 5.2, we have used language pre-trained DeBERTa for graph isomorphism learning, even though the records of random walks do not resemble natural language (Appendix A.2 and A.3). To test if language pre-training is useful, we additionally trained RWNN-DeBERTa on CSL and SR16 datasets using the same configurations to our reported models but from random initialization. The training curves are given in Figure 14. We find that pre-training has significant benefits over random initialization for isomorphism learning tasks, as randomly initialized models converge very slowly for CSL, and fails to converge to near-zero training loss for SR16.

Table 6: Fine-tuning for arXiv, extending Table 4. † denotes using validation labels as in Table 4.

Method	Training-free?	Accuracy
Llama3-8b zero-shot	◯	50.20%
Llama3-8b one-shot	◯	52.49%
Llama3-8b one-shot†	◯	52.54%
Llama3-70b zero-shot	◯	65.33%
Llama3-70b one-shot	◯	67.57%
RWNN-Llama3-8b (Ours)	◯	71.10%
RWNN-Llama3-8b (Ours)†	◯	73.11%
RWNN-Llama3-70b (Ours)†	◯	74.75%
RWNN-Llama3-8b (Ours), LoRA	×	**74.95%**

Table 7: Real-world transductive classification test accuracy on several homophilic (Cora, Citeseer) and heterophilic (Amazon Ratings) datasets. The baseline results were collected from (Sato, 2024; Zhao et al., 2023; Chen et al., 2024a; Liu et al., 2024; Chen et al., 2024b; Platonov et al., 2023). † denotes using validation labels as in Table 4.

Method	Training-free?	Cora 20-shot	Cora	Citeseer	Amazon Ratings
Training-free GNN	◯	60.00%	-	-	-
GCN	×	81.40%	89.13%	74.92%	48.70%
GAT	×	80.80%	89.68%	75.39%	49.09%
GraphText	◯	68.30%	67.77%	68.98%	-
LLaGA	◯	-	59.59%	-	-
GraphText	×	-	87.11%	74.77%	-
LLaGA	×	-	88.86%	-	28.20%
OFA	×	75.90%	-	-	51.44%
RWNN-Llama3-8b (Ours)	◯	72.05%	86.72%	78.37%	44.29%
RWNN-Llama3-8b (Ours)†	◯	79.40%	88.01%	78.53%	48.83%
RWNN-Llama3-8b (Ours), LoRA	×	79.45%	86.72%	81.03%	53.90%

A.4.2 Real-world Graph Classification

We conduct a preliminary experiment on the Peptides-func dataset (Dwivedi et al., 2022) used in Tönshoff et al. (2023). Our model is a pre-trained DeBERTa-base (identical to Section 5.2) fine-tuned on text records of non-backtracking MDLR random walks with anonymization and neighborhood recording. The recording function is designed to properly incorporate the vertex and edge attributes provided in the dataset, including the atom and bond types. An example text is provided in Figure 15.

In Table 5, we report the test average precision (AP) at best validation accuracy, with 40 random predicted logits averaged at test time. We report the mean and standard deviation of the test performances for five repeated tests. The baseline scores, including CRaWl, are from Tönshoff et al. (2023). We see that RWNN-DeBERTa, which has been successful in graph isomorphism learning (Section 5.2), also shows a promising result in real-world protein graph classification, despite its simplicity of recording random walks in text and processing them with a fine-tuned language model.

A.4.3 Fine-tuning for arXiv Transductive Classification (Section 5.3)

In Section 5.3, our RWNNs are training-free. We provide a preliminary result on fine-tuning on training labels using low-rank adaptation (LoRA) (Hu et al., 2022). The result is in Table 6, showing a promising performance.

A.4.4 Additional Real-world Transductive Classification

We provide additional experiments on real-world transductive classification datasets Cora, Citeseer, and Amazon Ratings. Our models are similar to ones in Section 5.3. We compile the baseline scores from (Zhao et al., 2023; Chen et al., 2024a; Liu et al., 2024; Chen et al., 2024b; Platonov et al., 2023), including MPNNs and language models on graphs. The results are in Table 7. Ours is competitive as a training-free method, and is reasonably good when fine-tuned with LoRA. Especially, on Amazon Ratings which is heterophilic (Platonov et al., 2023), our fine-tuned model outperforms all baselines.

Table 8: Substructure (8-cycle) counting. We report normalized test mean absolute error (MAE) at best validation. We trained MP, Subgraph GNN, Local 2-GNN, and Local 2-FGNN using configurations in Zhang et al. (2024), and trained MP-RNI, MP-Dropout, AgentNet, and CRaWl as in Table 3.

Method	Graph-level	Vertex-level
MP	.0917	.1156
Subgraph GNN	.0515	.0715
Local 2-GNN	.0433	.0478
Local 2-FGNN	.0422	.0438
Local 2-FGNN (large)	.0932	.1121
MP-RNI	.3610	.3650
MP-Dropout	.1359	.1393
AgentNet	.1107	N/A
CRaWl	.0526	.0725
RWNN-DeBERTa (Ours)	.0459	.0465

Table 9: Real-world link prediction. The baseline scores are from Table 5 of Cai et al. (2021), and we reproduced LGLP ourselves. We report the aggregated test AP for 3 randomized runs.

Method	YST	KHN	ADV
Katz	81.63 ± 0.41	83.04 ± 0.38	91.76 ± 0.15
PR	82.08 ± 0.46	87.18 ± 0.26	92.43 ± 0.17
SR	76.02 ± 0.49	75.87 ± 0.66	83.22 ± 0.20
node2vec	76.61 ± 0.94	80.60 ± 0.74	76.70 ± 0.82
SEAL	86.45 ± 0.25	90.37 ± 0.16	93.52 ± 0.13
LGLP	88.54 ± 0.77	90.80 ± 0.33	93.51 ± 0.32
RWNN-transformer (Ours)	88.18 ± 0.28	90.63 ± 0.44	93.52 ± 0.20

This supports our results in Section 3.2 that RWNNs avoid over-smoothing, as avoiding it is known to be important for handling heterophily (Yan et al., 2022).

A.4.5 Substructure Counting

We test RWNN on additional challenging tasks that require both expressive power and generalization to unseen graphs. We use a synthetic dataset of 5,000 random regular graphs from Chen et al. (2020), and consider the task of counting substructures. We choose 8-cycles since they are known to require a particularly high expressive power (Zhang et al., 2024). We experiment with both graph- and vertex-level counting i.e. counting 8-cycles containing the queried vertex, following Zhang et al. (2024). We use the data splits from previous work (Chen et al., 2020; Zhao et al., 2022b; Zhang et al., 2024), while excluding disconnected graphs following our modeling assumption in Section 2.1. Our RWNN uses the same design to Section 5.2, and we train them with L1 loss for at most 250k steps using batch size of 128 graphs for graph-level counting and 8 graphs for vertex-level. At test-time, we ensemble 64 and 32 predictions by averaging for graph- and vertex-level tasks, respectively.

The results are in Table 8, and overall in line with Section 5.2. While MPNNs show a low performance, variants with higher expressive powers such as local 2-GNN and local 2-FGNN achieve high performances. This is consistent with the observation of Zhang et al. (2024). On the other hand, MPNNs with stochastic symmetry-breaking often show learning difficulties and does not achieve good performance. AgentNet was not directly applicable for vertex-level counting since its vertex encoding depends on which vertices the agent visits, and a learning difficulty was observed for graph-level counting. Our approach based on DeBERTa demonstrates competitive performance, outperforming random walk baselines and approaching performances of local 2-GNN and 2-FGNN.

A.4.6 Link Prediction

We test an extension to real-world link prediction, based on Cai et al. (2021) where link prediction is cast as vertex classification on a line graph. We follow Cai et al. (2021) and only change their 3-layer 32-dim DGCNN with an RWNN that uses a 3-layer 32-dim transformer encoder. As the task is vertex-level, we use periodic restarts with $k = 4$. The results in Table 9 shows that RWNN performs reasonably well.

A.5 PROOFS

We recall that an isomorphism between two graphs G and H is a bijection $\pi : V(G) \to V(H)$ such that any two vertices u and v are adjacent in G if and only if $\pi(u)$ and $\pi(v)$ are adjacent in H. If an isomorphism π exists between G and H, the graphs are isomorphic and written $G \simeq H$ or $G \overset{\pi}{\simeq} H$. By $X \overset{d}{=} Y$ we denote the equality of two random variables X and Y in distributions.

In the proofs, we write by $\mathrm{id}(\cdot)$ the namespace obtained by anonymization of a walk $v_0 \to \cdots \to v_l$ (Section 2) that maps each vertex v_t to its unique integer name $\mathrm{id}(v_t)$ starting from $\mathrm{id}(v_0) = 1$.

Let us define some notations related to cover times. These will be used from Appendix A.5.5. We denote by $H(u, v)$ the expected number of steps a random walk starting from u takes until reaching v. This is called the hitting time between u and v. For a graph G, let $C_V(G, u)$ be the expected number of steps a random walk starting from u takes until visiting every vertices of G. The vertex cover time $C_V(G)$, or the cover time, is this quantity given by the worst possible u:

$$C_V(G) \coloneqq \max_{u \in V(G)} C_V(G, u). \tag{16}$$

Likewise, let $C_E(G, u)$ be the expected number of steps a random walk starting from u takes until traversing every edge of G. The edge cover time $C_E(G)$ is given by the worst possible u:

$$C_E(G) \coloneqq \max_{u \in V(G)} C_E(G, u). \tag{17}$$

For local balls $B_r(u)$, we always set the starting vertex of the random walk to u (Section 2.2). Thus, we define their cover times as follows:

$$C_V(B_r(u)) \coloneqq C_V(B_r(u), u), \tag{18}$$
$$C_E(B_r(u)) \coloneqq C_E(B_r(u), u). \tag{19}$$

A.5.1 PROOF OF PROPOSITION 2.1 (SECTION 2)

Proposition 2.1. *$X_\theta(\cdot)$ is invariant in probability, if its random walk algorithm is invariant in probability and its recording function is invariant.*

Proof. We recall the probabilistic invariance of random walk algorithm in Equation 3:

$$\pi(v_0) \to \cdots \to \pi(v_l) \overset{d}{=} u_0 \to \cdots \to u_l, \quad \forall G \overset{\pi}{\simeq} H, \tag{20}$$

where $v_{[\cdot]}$ is a random walk on G and $u_{[\cdot]}$ is a random walk on H. We further recall the invariance of recording function $q : (v_0 \to \cdots \to v_l, G) \mapsto \mathbf{z}$ in Equation 7:

$$q(v_0 \to \cdots \to v_l, G) = q(\pi(v_0) \to \cdots \to \pi(v_l), H), \quad \forall G \overset{\pi}{\simeq} H, \tag{21}$$

for any given random walk $v_{[\cdot]}$ on G. Combining Equation 20 and equation 21, we have the following:

$$q(v_0 \to \cdots \to v_l, G) \overset{d}{=} q(u_0 \to \cdots \to u_l, H), \quad \forall G \simeq H. \tag{22}$$

Then, since the reader neural network f_θ is a deterministic map, we have:

$$f_\theta(q(v_0 \to \cdots \to v_l, G)) \overset{d}{=} f_\theta(q(u_0 \to \cdots \to u_l, H)), \quad \forall G \simeq H, \tag{23}$$

which leads to:

$$X_\theta(G) \overset{d}{=} X_\theta(H), \quad \forall G \simeq H. \tag{24}$$

This shows Equation 2 and completes the proof. □

A.5.2 PROOF OF PROPOSITION 2.2 (SECTION 2)

We first show a useful lemma.

Lemma A.2. *The random walk in Equation 4 is invariant in probability, if the probability distributions of the starting vertex v_0 and each transition $v_{t-1} \to v_t$ are invariant.*

Proof. We prove by induction. Let us write probabilistic invariance of the starting vertex v_0 as:

$$\pi(v_0) \overset{d}{=} u_0, \quad \forall G \overset{\pi}{\simeq} H, \tag{25}$$

and probabilistic invariance of each transition $v_{t-1} \to v_t$ as follows, by fixing v_{t-1} and u_{t-1}:

$$\pi(v_{t-1}) \to \pi(v_t) \overset{d}{=} u_{t-1} \to u_t, \quad \forall G \overset{\pi}{\simeq} H, v_{t-1} \in V(G), u_{t-1} \coloneqq \pi(v_{t-1}). \tag{26}$$

Let us assume the following for some $t \geq 1$:

$$\pi(v_0) \to \cdots \to \pi(v_{t-1}) \overset{d}{=} u_0 \to \cdots \to u_{t-1}, \quad G \overset{\pi}{\simeq} H. \tag{27}$$

Then, from the chain rule of joint distributions, the first-order Markov property of random walk in Equation 4, and probabilistic invariance in Equation 26, we obtain the following:

$$\pi(v_0) \to \cdots \to \pi(v_t) \overset{d}{=} u_0 \to \cdots \to u_t, \quad G \overset{\pi}{\simeq} H. \tag{28}$$

By induction from the initial condition $\pi(v_0) \overset{d}{=} u_0$ in Equation 25, the following holds $\forall l > 0$:

$$\pi(v_0) \to \cdots \to \pi(v_l) \overset{d}{=} u_0 \to \cdots \to u_l, \quad \forall G \overset{\pi}{\simeq} H. \tag{29}$$

This shows Equation 3 and completes the proof. □

We now prove Proposition 2.2.

Proposition 2.2. *The random walk in Equation 4 is invariant in probability if its conductance $c_{[\cdot]}(\cdot)$ is invariant:*

$$c_G(u, v) = c_H(\pi(u), \pi(v)), \quad \forall G \overset{\pi}{\simeq} H. \tag{30}$$

It includes constant conductance, and any choice that only uses degrees of endpoints $\deg(u)$, $\deg(v)$.

Proof. We recall Equation 4 for a given conductance function $c_G : E(G) \to \mathbb{R}_+$:

$$\mathrm{Prob}[v_t = x | v_{t-1} = u] \coloneqq \frac{c_G(u, x)}{\sum_{y \in N(u)} c_G(u, y)}. \tag{31}$$

From Lemma A.2, it is sufficient to show the probabilistic invariance of each transition $v_{t-1} \to v_t$ as we sample v_0 from invariant distribution $\mathrm{Uniform}(V(G))$ (Algorithm 1). We rewrite Equation 26 as:

$$\mathrm{Prob}[v_t = x | v_{t-1} = u] = \mathrm{Prob}[u_t = \pi(x) | u_{t-1} = \pi(u)], \quad \forall G \overset{\pi}{\simeq} H. \tag{32}$$

If the conductance function $c_{[\cdot]}(\cdot)$ is invariant (Equation 30), we can show Equation 32 by:

$$\begin{aligned}
\mathrm{Prob}[v_t = x | v_{t-1} = u] &\coloneqq \frac{c_G(u, x)}{\sum_{y \in N(u)} c_G(u, y)}, \\
&= \frac{c_H(\pi(u), \pi(x))}{\sum_{y \in N(u)} c_H(\pi(u), \pi(y))}, \\
&= \frac{c_H(\pi(u), \pi(x))}{\sum_{\pi(y) \in N(\pi(u))} c_H(\pi(u), \pi(y))}, \\
&= \mathrm{Prob}[u_t = \pi(x) | u_{t-1} = \pi(u)], \quad \forall G \overset{\pi}{\simeq} H.
\end{aligned} \tag{33}$$

In the third equality, we used the fact that isomorphism $\pi(\cdot)$ preserves adjacency. It is clear that any conductance function $c_{[\cdot]}(\cdot)$ with a constant conductance such as $c_G(\cdot) = 1$ is invariant. Furthermore, any conductance function that only uses degrees of endpoints $\deg(u)$, $\deg(v)$ is invariant as isomorphism $\pi(\cdot)$ preserves the degree of each vertex. This completes the proof. □

A.5.3 Proof of Proposition A.1 (Appendix A.1)

We extend the proof of Proposition 2.2 given in Appendix A.5.2 to second-order random walks discussed in Appendix A.1. We first show a useful lemma:

Lemma A.3. *A second-order random walk algorithm is invariant in probability, if the probability distributions of the starting vertex v_0, the first transition $v_0 \to v_1$, and each transition $(v_{t-2}, v_{t-1}) \to v_t$ for $t > 1$ are invariant.*

Proof. We prove by induction. The probabilistic invariance of starting vertex v_0 and first transition $v_0 \to v_1$ are:

$$\pi(v_0) \overset{d}{=} u_0, \quad \forall G \overset{\pi}{\simeq} H, \tag{34}$$

$$\pi(v_0) \to \pi(v_1) \overset{d}{=} u_0 \to u_1, \quad \forall G \overset{\pi}{\simeq} H, v_0 \in V(G), u_0 \coloneqq \pi(v_0), \tag{35}$$

and probabilistic invariance of each transition $(v_{t-2}, v_{t-1}) \to v_t$ for $t > 1$ can be written as follows by fixing (v_{t-2}, v_{t-1}) and (u_{t-2}, u_{t-1}):

$$\begin{aligned} \pi(v_{t-2}) \to \pi(v_{t-1}) \to \pi(v_t) \overset{d}{=} u_{t-2} \to u_{t-1} \to u_t, \quad & \forall G \overset{\pi}{\simeq} H, \\ & (v_{t-2}, v_{t-1}) \in E(G), \\ & (u_{t-2}, u_{t-1}) \coloneqq (\pi(v_{t-2}), \pi(v_{t-1})). \end{aligned} \tag{36}$$

Let us assume the following for some $t \geq 2$:

$$\pi(v_0) \to \cdots \to \pi(v_{t-2}) \to \pi(v_{t-1}) \overset{d}{=} u_0 \to \cdots \to u_{t-2} \to u_{t-1}, \quad G \overset{\pi}{\simeq} H. \tag{37}$$

Then, from the chain rule of joint distributions, the second-order Markov property of second-order random walks, and probabilistic invariance in Equation 36, we obtain the following:

$$\pi(v_0) \to \cdots \to \pi(v_{t-1}) \to \pi(v_t) \overset{d}{=} u_0 \to \cdots \to u_{t-1} \to u_t, \quad G \overset{\pi}{\simeq} H. \tag{38}$$

By induction from the initial condition $\pi(v_0) \to \pi(v_1) \overset{d}{=} u_0 \to u_1$ given from Equations 34 and 35, the following holds $\forall l > 0$:

$$\pi(v_0) \to \cdots \to \pi(v_l) \overset{d}{=} u_0 \to \cdots \to u_l, \quad \forall G \overset{\pi}{\simeq} H. \tag{39}$$

This shows Equation 3 and completes the proof. □

We now prove Proposition A.1.

Proposition A.1. *The non-backtracking random walk in Equation 13 and the node2vec random walk in Equation 14 are invariant in probability, if their underlying first-order random walk algorithm is invariant in probability.*

Proof. We assume that the first transition $v_0 \to v_1$ is given by the underlying first-order random walk algorithm. This is true for non-backtracking since there is no v_{t-2} to avoid, and true for the official implementation of node2vec (Grover & Leskovec, 2016). Then from Lemma A.3, it is sufficient to show probabilistic invariance of each transition $(v_{t-2}, v_{t-1}) \to v_t$ for $t > 1$ as we sample v_0 from the invariant distribution $\mathrm{Uniform}(V(G))$ (Algorithm 1) and the first transition $v_0 \to v_1$ is given by the first-order random walk which is assumed to be invariant in probability. Rewrite Equation 36 as:

$$\mathrm{Prob}[v_t = x | v_{t-1} = j, v_{t-2} = i] = \mathrm{Prob}[u_t = \pi(x) | u_{t-1} = \pi(j), u_{t-2} = \pi(i)], \quad \forall G \overset{\pi}{\simeq} H. \tag{40}$$

For non-backtracking, we first handle the case where $i \to j$ reaches a dangling vertex j which has i as its only neighbor. In this case the walk begrudgingly backtracks $i \to j \to i$ (Appendix A.1). Since isomorphism $\pi(\cdot)$ preserves adjacency, $\pi(i) \to \pi(j)$ also reaches a dangling vertex $\pi(j)$ and must begrudgingly backtrack $\pi(i) \to \pi(j) \to \pi(i)$. By interpreting the distributions on v_t and u_t as one-hot at i and $\pi(i)$, respectively, we can see that Equation 40 holds. If $i \to j$ does not reach a

dangling vertex, the walk $j \to x$ follows the invariant probability of the underlying first-order random walk $\mathrm{Prob}[v_{t+1} = x | v_t = j]$ renormalized over $N(j) \setminus \{i\}$. Then we can show Equation 40 by:

$$\begin{aligned}
&\mathrm{Prob}[v_t = x | v_{t-1} = j, v_{t-2} = i] \\
&\qquad := \begin{cases} \dfrac{\mathrm{Prob}[v_t = x | v_{t-1} = j]}{\sum_{y \in N(j) \setminus \{i\}} \mathrm{Prob}[v_t = y | v_{t-1} = j]} & \text{for } x \neq i, \\ 0 & \text{for } x = i, \end{cases} \\
&\qquad = \begin{cases} \dfrac{\mathrm{Prob}[u_t = \pi(x) | u_{t-1} = \pi(j)]}{\sum_{\pi(y) \in N(\pi(j)) \setminus \{\pi(i)\}} \mathrm{Prob}[u_t = \pi(y) | u_{t-1} = \pi(j)]} & \text{for } \pi(x) \neq \pi(i), \\ 0 & \text{for } \pi(x) = \pi(i), \end{cases} \\
&\qquad = \mathrm{Prob}[u_t = \pi(x) | u_{t-1} = \pi(j), u_{t-2} = \pi(i)], \quad \forall G \overset{\pi}{\simeq} H. \qquad (41)
\end{aligned}$$

In the second equality, we have used the fact that isomorphism $\pi(\cdot)$ is a bijection and preserves adjacency, and the assumption that the first-order random walk algorithm is invariant in probability. For node2vec walk, we first show the invariance of the weighting term $\alpha(i, x)$ in Equation 15 using the fact that isomorphism preserves shortest path distances between vertices $d(i, x) = d(\pi(i), \pi(x))$:

$$\begin{aligned}
\alpha(i, x) &:= \begin{cases} 1/p & \text{for } d(i, x) = 0, \\ 1 & \text{for } d(i, x) = 1, \\ 1/q & \text{for } d(i, x) = 2. \end{cases} \\
&= \begin{cases} 1/p & \text{for } d(\pi(i), \pi(x)) = 0, \\ 1 & \text{for } d(\pi(i), \pi(x)) = 1, \\ 1/q & \text{for } d(\pi(i), \pi(x)) = 2. \end{cases} \\
&= \alpha(\pi(i), \pi(x)). \qquad (42)
\end{aligned}$$

Then we can show Equation 40 by:

$$\begin{aligned}
\mathrm{Prob}[v_t = x | v_{t-1} = j, v_{t-2} = i] &:= \frac{\alpha(i, x) \, \mathrm{Prob}[v_t = x | v_{t-1} = j]}{\sum_{y \in N(j)} \alpha(i, y) \, \mathrm{Prob}[v_t = y | v_{t-1} = j]}, \\
&= \frac{\alpha(\pi(i), \pi(x)) \, \mathrm{Prob}[u_t = \pi(x) | u_{t-1} = \pi(j)]}{\sum_{\pi(y) \in N(\pi(j))} \alpha(\pi(i), \pi(y)) \, \mathrm{Prob}[u_t = \pi(y) | u_{t-1} = \pi(j)]}, \\
&= \mathrm{Prob}[u_t = \pi(x) | u_{t-1} = \pi(j), u_{t-2} = \pi(i)], \quad \forall G \overset{\pi}{\simeq} H. \qquad (43)
\end{aligned}$$

In the second equality, we have used the fact that isomorphism $\pi(\cdot)$ preserves adjacency, and the assumption that the first-order walk algorithm is invariant in probability. This completes the proof. □

A.5.4 Proof of Proposition 2.3 (Section 2)

Proposition 2.3. *A recording function $q : (v_0 \to \cdots \to v_l, G) \mapsto \mathbf{z}$ that uses anonymization, optionally with named neighbors, is invariant.*

Proof. Given a walk $v_0 \to \cdots \to v_l$ on G, we can write the anonymized namespace $\mathrm{id}(\cdot)$ as follows:

$$\mathrm{id}(v_t) = 1 + \arg\min_i [v_i = v_t]. \qquad (44)$$

Consider any walk $\pi(v_0) \to \cdots \to \pi(v_l)$ on some H which is isomorphic to G via π. Let us denote the anonymization of this walk as $\mathrm{id}'(\cdot)$. Then we have:

$$\begin{aligned}
\mathrm{id}'(\pi(v_t)) &= 1 + \arg\min_i [\pi(v_i) = \pi(v_t)], \\
&= 1 + \arg\min_i [v_i = v_t], \\
&= \mathrm{id}(v_t), \quad \forall G \overset{\pi}{\simeq} H. \qquad (45)
\end{aligned}$$

The second equality is due to the fact that π is a bijection. This completes the proof for anonymization. For the named neighbors, we prove by induction. Let us fix some $t \geq 1$ and assume:

$$q(v_0 \to \cdots \to v_{t-1}, G) = q(\pi(v_0) \to \cdots \to \pi(v_{t-1}), H), \quad \forall G \overset{\pi}{\simeq} H. \tag{46}$$

Let $T \subseteq E(G)$ be the set of edges recorded by $\mathbf{z} \coloneqq q(v_0 \to \cdots \to v_{t-1}, G)$, and $T' \subseteq E(H)$ be the set of edges recorded by $\mathbf{z}' \coloneqq q(\pi(v_0) \to \cdots \to \pi(v_{t-1}), H)$. Then, T and T' are isomorphic via π:

$$T' = \{(\pi(u), \pi(v)) \forall (u, v) \in T\}. \tag{47}$$

The equality is shown as follows. ($\supseteq$) Any $(u, v) \in T$ is recorded in $\mathbf{z}$ as $(\mathrm{id}(u), \mathrm{id}(v))$. From Equations 46 and 45, we have $\mathbf{z} = \mathbf{z}'$ and $(\mathrm{id}(u), \mathrm{id}(v)) = (\mathrm{id}(\pi(u)), \mathrm{id}(\pi(v)))$. Thus, $(\pi(u), \pi(v))$ is recorded in $\mathbf{z}'$ as $(\mathrm{id}(\pi(u)), \mathrm{id}(\pi(v)))$, i.e. $(\pi(u), \pi(v)) \in T'$. ($\subseteq$) This follows from symmetry. Now, we choose some $v_t \in N(v_{t-1})$ and consider the set $F \subseteq E(G)$ of all unrecorded edges from v_t:

$$F \coloneqq \{(v_t, u) : u \in N(v_t)\} \setminus T. \tag{48}$$

Then, the set D of unrecorded neighbors of v_t is given as:

$$D \coloneqq \{u : (v_t, u) \in F\}. \tag{49}$$

Since $\pi(\cdot)$ preserves adjacency, the set $F' \subseteq E(H)$ of all unrecorded edges from $\pi(v_t)$ is given by:

$$\begin{aligned} F' &\coloneqq \{(\pi(v_t), \pi(u)) : \pi(u) \in N(\pi(v_t))\} \setminus T', \\ &= \{(\pi(v_t), \pi(u)) : u \in N(v_t)\} \setminus \{(\pi(u'), \pi(v')) \forall (u', v') \in T\}, \\ &= \{(\pi(v_t), \pi(u)) : u \in N(v_t), (v_t, u) \notin T\}, \\ &= \{(\pi(v_t), \pi(u)) : (v_t, u) \in F\}, \end{aligned} \tag{50}$$

and consequently:

$$\begin{aligned} D' &\coloneqq \{\pi(u) : (\pi(v_t), \pi(u)) \in F'\}, \\ &= \{\pi(u) : u \in D\}. \end{aligned} \tag{51}$$

While D and D' may contain vertices not yet visited by the walks and hence not named by $\mathrm{id}(\cdot)$, what we record are named neighbors. Let S be the set of all named vertices in G. It is clear that the set S' of named vertices in H is given by $S' = \{\pi(v) : v \in S\}$. Then, the named neighbors in G to be newly recorded for $v_{t-1} \to v_t$ is given by $U = D \cap S$, and for $\pi(v_{t-1}) \to \pi(v_t)$ in H the set is given by $U' = D' \cap S'$. Since $\pi(\cdot)$ is a bijection, we can see that $U' = \{\pi(u) : u \in U\}$. From the invariance of anonymization in Equation 45, U and U' are named identically $\{\mathrm{id}(u) : u \in U\} = \{\mathrm{id}(\pi(u)) : \pi(u) \in U'\}$, and therefore will be recorded identically. As a result, the information to be added to the records at time t are identical, and we have:

$$q(v_0 \to \cdots \to v_t, G) = q(\pi(v_0) \to \cdots \to \pi(v_t), H), \quad \forall G \overset{\pi}{\simeq} H. \tag{52}$$

Then, by induction from the initial condition:

$$q(v_0, G) = q(\pi(v_0), H) = \mathrm{id}(v_0) = \mathrm{id}(\pi(v_0)) = 1, \tag{53}$$

the recording function using anonymization and named neighbors is invariant. □

A.5.5 Proof of Theorem 2.4 (Section 2.2)

Theorem 2.4. *For a uniform random walk on an infinite graph G starting at v, the vertex and edge cover times of the finite local ball $B_r(v)$ are not always finitely bounded.*

Proof. We revisit the known fact that hitting times on the infinite line $\mathbb{Z}$ is infinite (Dumitriu et al., 2003; Janson & Peres, 2012; carnage, 2012; McNew, 2013). Consider a local ball $B_1(0)$ of radius 1 from the origin 0 such that $V(B_1(0)) = \{-1, 0, 1\}$. Let us assume that the expected number of steps for a random walk starting at 0 to visit 1 for the first time is finite, and denote it by T. In the first step of the walk, we have to go either to -1 or 1. If we go to -1, we have to get back to 0 and then to 1 which would take $2T$ in expectation (by translation symmetry). This leads to $T = 1/2 \cdot 1 + 1/2 \cdot (1 + 2T) = 1 + T$, which is a contradiction. Since visiting all vertices or traversing all edges in in $B_1(0)$ clearly involves visiting 1, the vertex and edge cover times cannot be finitely bounded. □

A.5.6 PROOF OF THEOREM 2.5 (SECTION 2.2)

Let us recall that our graph G is locally finite (Section 2.2), and denote its maximum degree as Δ. We further denote by $d(u, v)$ the shortest path distance between u and v. We show some useful lemmas. We first show that $H(u, x)$, the expected number of steps of a random walk starting at u takes until reaching x, is finite for any u, x in $B_r(v)$ for any nonzero restart probability α or restart period $k \geq r$.

Lemma A.4. *For any u and x in $B_r(v)$, $H(u, x)$ is bounded by the following:*

$$H(u,x) \leq \frac{1}{\alpha} + \frac{1}{\alpha}\left(\frac{\Delta}{1-\alpha}\right)^r + \frac{1}{\alpha}\left(\frac{1}{\alpha} - 1\right)\left(\frac{\Delta}{1-\alpha}\right)^{2r}, \tag{54}$$

if the random walk restarts at v with any probability $\alpha \in (0, 1)$, and:

$$H(u,x) \leq k + k\Delta^r, \tag{55}$$

if the random walk restarts at v with any period $k \geq r$.

Proof. We first prove for random restarts. The proof is inspired by Theorem 1.1 of McNew (2013) and Lemma 2 of Zuckerman (1991). We clarify some measure-theoretic details. Let W be the set of all (infinite) random walks on G. We denote by P the probability measure defined on the space W, equipped with its cylinder σ-algebra, by the random walk restarting at v with probability $\alpha \in (0, 1)$. For a vertex x in G, we define the hitting time function $|\cdot|_x : W \to \mathbb{N} \cup \{\infty\}$ as follows:

$$|w|_x \coloneqq \arg\min_i [(w)_i = x], \quad \forall w \in W. \tag{56}$$

Let $W(a)$ be the set of all random walks that start at a, $W(a, b)$ be the set of random walks that start at a and visit b, and $W(a, b^-)$ be the set of random walks that start at a and do not visit b. Then, the measurability of $|\cdot|_x$ follows from the measurability of the sets $W(a)$, $W(a, b)$, and $W(a, b^-)$, which we show as follows. $\forall a, b \in V(G)$, $W(a)$ is clearly measurable, $W(a, b)$ is measurable as it equals $\bigcup_{n\in\mathbb{N}}\{w \in W | (w)_1 = a, (w)_n = b\}$, and $W(a, b^-)$ is measurable as it is $W(a) \setminus W(a, b)$.

Consider $W(u, x^-)$, the set of random walks that start at u and never visit x. We start by showing that this set is of measure zero:

$$P(W(u, x^-)) = 0. \tag{57}$$

For this, we use the fact that $W(u, x^-) = W(u, v^-, x^-) \cup W(u, v, x^-)$, where $W(u, v^-, x^-)$ is the set of random walks starting at u that do not visit v nor x, and $W(u, v, x^-)$ is the set of walks starting at u that visit v and do not visit x. We have the following:

$$\begin{aligned} P(W(u, x^-)) &= P(W(u, v^-, x^-)) + P(W(u, v, x^-)), \\ &\leq P(W(u, v^-)) + P(W(u, v, x^-)). \end{aligned} \tag{58}$$

We show Equation 57 by showing $P(W(u, v^-)) = 0$ and $P(W(u, v, x^-)) = 0$ in Equation 58.

1. $(P(W(u, v^-)) = 0)$ Consider $W(u, v^-)$, the set of all random walks that start at u and never visit v. Since restart sends a walk to v, every walk in this set never restarts. The probability of a walk not restarting until step t is $(1 - \alpha)^t$. Denote this probability by p_t, and let p be the probability of a random walk to never restart. Then $p_t \downarrow p = 0$ and $P(W(u, v^-)) \leq p = 0$.
2. $(P(W(u, v, x^-)) = 0)$ Assume $P(W(u, v, x^-)) > 0$. Then $P(W(v, x^-)) > 0$ since each walk step is independent. Let $W_N(v, x^-)$ be the set of walks that start at v and do not reach x within N restarts. Then we have $W_N(v, x^-) \downarrow W(v, x^-)$. If a walk restarts at v, the probability of reaching x before the next restart is at least the probability of exactly walking the shortest path from v to x, which is $\geq (\frac{1-\alpha}{\Delta})^{d(v,x)} \in (0, 1)$. Then $P(W_N(v, x^-)) \leq (1 - (\frac{1-\alpha}{\Delta})^{d(v,x)})^N \downarrow 0$, leading to $P(W(v, x^-)) = 0$. This is a contradiction, so we have $P(W(u, v, x^-)) = 0$.

We are now ready to bound $H(u, x)$. Using the hitting time function $|\cdot|_x$ in Equation 56, we have:

$$H(u,x) = \mathbb{E}\left[|w|_x | w \in W(u)\right]. \tag{59}$$

Since $W(u) = W(u,x) \cup W(u,x^-)$, and $P(W(u,x^-)) = 0$ from Equation 57, we have:

$$\begin{aligned} H(u,x) &= \mathbb{E}[|w|_x | w \in W(u,x)], \\ &= \int_{W(u,x)} |w|_x \, dP(w | w \in W(u,x)). \end{aligned} \tag{60}$$

Each walk in $W(u,x)$ starts at u and, when it reaches x, it either has or has not visited v. We treat the two cases separately. Let $W(a,b,c)$ be the set of walks that start at a and reach c after b, and let $W(a,b^-,c)$ be the set of walks that start at a and reach c before b. Then we have:

$$\begin{aligned} H(u,x) &= \int_{W(u,v,x) \cup W(u,v^-,x)} |w|_x \, dP(w|W(u,x)), \\ &= \int_{W(u,v,x)} |w|_x \, dP(w|W(u,x)) + \int_{W(u,v^-,x)} |w|_x \, dP(w|W(u,x)). \end{aligned} \tag{61}$$

Let $\hat{H}(a,b,c)$ (or $\hat{H}(a,b^-,c)$) be the expected number of steps for a walk starting at a to reach c after reaching b (or before b), given that it is in $W(a,b,c)$ (or in $W(a,b^-,c)$). If a walk from u reaches v before x, the expected steps is given by $\hat{H}(u,x^-,v) + H(v,x)$. If the walk reaches x before v, the expected steps is $\hat{H}(u,v^-,x)$. Then, if $W(u,v^-,x) \neq \emptyset$, we can write $H(u,x)$ as follows:

$$\begin{aligned} H(u,x) = &\left[\hat{H}(u,x^-,v) + H(v,x)\right] P(W(u,v,x)|W(u,x)) \\ &+ \hat{H}(u,v^-,x) \, P(W(u,v^-,x)|W(u,x)). \end{aligned} \tag{62}$$

On the other hand, if $W(u,v^-,x) = \emptyset$, we simply have:

$$H(u,x) = \hat{H}(u,x^-,v) + H(v,x). \tag{63}$$

We first consider $\hat{H}(u,x^-,v)$, the expected number of steps from u to reach v before x. We show:

$$\hat{H}(u,x^-,v) \leq \frac{1}{\alpha}. \tag{64}$$

To see this, note that $\hat{H}(u,x^-,v)$ is equivalent to the expectation $\mathbb{E}[T]$ of the number of steps T to reach v from u, on the graph G with the vertex x deleted and transition probabilities renormalized. If u is isolated on this modified graph, the only walk in $W(u,x^-,v)$ is the one that immediately restarts at v, giving $\mathbb{E}[T] = 1$. Otherwise, we have $\mathbb{E}[T] \leq 1/\alpha$ due to the following. Let T' be the number of steps until the first restart at v. Since restart can be treated as a Bernoulli trial with probability of success α, T' follows geometric distribution with expectation $1/\alpha$. Since it is possible for the walk to reach v before the first restart, we have $\mathbb{E}[T] \leq \mathbb{E}[T'] = 1/\alpha$, which gives Equation 64.

We now consider $H(v,x)$, the expectation $\mathbb{E}[T]$ of the number of steps T to reach x from v. Let T' be the steps until the walk restarts at v, then exactly walks the shortest path from v to x for the first time, and then restarts at v. Since T' walks until restart after walking the shortest path to x, and it is possible for a walk to reach x before walking the shortest path to it, we have $\mathbb{E}[T] \leq \mathbb{E}[T']$. Then, we split the walk of length T' into N trials, where each trial consists of restarting at v and walking until the next restart. A trial is successful if it immediately walks the shortest path from v to x. Then N is the number of trials until we succeed, and it follows geometric distribution with probability of success at least $(\frac{1-\alpha}{\Delta})^{d(v,x)}$ due to bounded degrees. Its expectation is then bounded as:

$$\mathbb{E}[N] \leq \left(\frac{\Delta}{1-\alpha}\right)^{d(v,x)}. \tag{65}$$

Let S_i be the length of the i-th trial. Since each S_i is i.i.d. with finite mean $\mathbb{E}[S_i] = 1/\alpha$, and N is stopping time, we can apply Wald's identity (Hein) to compute the expectation of T':

$$\begin{aligned} \mathbb{E}[T'] &= \mathbb{E}[S_1 + \cdots + S_N], \\ &= \mathbb{E}[N]\mathbb{E}[S_1], \\ &\leq \frac{1}{\alpha}\left(\frac{\Delta}{1-\alpha}\right)^{d(v,x)}. \end{aligned} \tag{66}$$

We remark that $H(v,x) \leq \mathbb{E}[T']$. Combining this result with Equation 64, we have:

$$\hat{H}(u,x^-,v) + H(v,x) \leq \frac{1}{\alpha} + \frac{1}{\alpha}\left(\frac{\Delta}{1-\alpha}\right)^{d(v,x)}. \tag{67}$$

If $W(u,v^-,x) = \emptyset$, we have $H(u,x) = \hat{H}(u,x^-,v) + H(v,x)$ from Equation 63 and it is finitely bounded for any $\alpha \in (0,1)$ by the above. If $W(u,v^-,x) \neq \emptyset$, Equations 62 and 67 lead to:

$$\begin{aligned} H(u,x) &\leq \hat{H}(u,x^-,v) + H(v,x) + \hat{H}(u,v^-,x)\, P(W(u,v^-,x)|W(u,x)), \\ &\leq \frac{1}{\alpha} + \frac{1}{\alpha}\left(\frac{\Delta}{1-\alpha}\right)^{d(v,x)} + \hat{H}(u,v^-,x)\, P(W(u,v^-,x)|W(u,x)), \end{aligned} \tag{68}$$

and it suffices to bound $\hat{H}(u,v^-,x)\, P(W(u,v^-,x)|W(u,x))$. We show the following:

$$\begin{aligned} \hat{H}(u,v^-,x) &= \int_{W(u,v^-,x)} |w|_x \, dP(w|W(u,v^-,x)), \\ &= \sum_{k=1}^{\infty} \int_{\{w \in W(u,v^-,x) \wedge |w|_x = k\}} |w|_x \, dP(w|W(u,v^-,x)), \\ &= \sum_{k=1}^{\infty} k \int_{\{w \in W(u,v^-,x) \wedge |w|_x = k\}} dP(w|W(u,v^-,x)), \\ &= \sum_{k=1}^{\infty} k\, P(\{w \in W(u,v^-,x) \wedge |w|_x = k\}|W(u,v^-,x)), \\ &\leq \sum_{k=1}^{\infty} k\, P(\{w : |w|_x = k\}|W(u,v^-,x)), \\ &= \sum_{k=1}^{\infty} k\, \frac{P(\{w : |w|_x = k \wedge w \in W(u,v^-,x)\})}{P(W(u,v^-,x))}, \\ &\leq \sum_{k=1}^{\infty} k(1-\alpha)^k \frac{1}{P(W(u,v^-,x))}, \\ &= \frac{1}{\alpha}\left(\frac{1}{\alpha} - 1\right) \frac{1}{P(W(u,v^-,x))}. \end{aligned} \tag{69}$$

We have used Fubini's theorem for the second equality. Then we have:

$$\begin{aligned} \hat{H}(u,v^-,x)\, P(W(u,v^-,x)|W(u,x)) &\leq \frac{1}{\alpha}\left(\frac{1}{\alpha} - 1\right) \frac{P(W(u,v^-,x)|W(u,x))}{P(W(u,v^-,x))}, \\ &= \frac{1}{\alpha}\left(\frac{1}{\alpha} - 1\right) \frac{1}{P(W(u,x))}. \end{aligned} \tag{70}$$

$P(W(u,x))$ is at least the probability of precisely walking the shortest path from u to x, which has length $d(u,x) \leq 2r$ since u and x are both in $B_r(v)$. This gives us the following:

$$\begin{aligned} P(W(u,x)) &\geq \left(\frac{1-\alpha}{\Delta}\right)^{d(u,x)}, \\ &\geq \left(\frac{1-\alpha}{\Delta}\right)^{2r}. \end{aligned} \tag{71}$$

Combining this with Equation 70, we have:

$$\hat{H}(u,v^-,x)\, P(W(u,v^-,x)|W(u,x)) \leq \frac{1}{\alpha}\left(\frac{1}{\alpha} - 1\right)\left(\frac{\Delta}{1-\alpha}\right)^{2r}. \tag{72}$$

Combining with Equations 62 and 67, we have:

$$H(u,x) \leq \frac{1}{\alpha} + \frac{1}{\alpha}\left(\frac{\Delta}{1-\alpha}\right)^{d(v,x)} + \frac{1}{\alpha}\left(\frac{1}{\alpha} - 1\right)\left(\frac{\Delta}{1-\alpha}\right)^{2r}, \tag{73}$$

for any $\alpha \in (0, 1)$. Notice that, while this bound is for the case $W(u, v^-, x) \neq \emptyset$, it subsumes the bound for the case $W(u, v^-, x) = \emptyset$ (Equation 67). Then, using $d(v, x) \leq r$, we get Equation 54. This completes the proof for random restarts.

We now prove for periodic restarts. If the walk starting at u reaches x before restarting at v, the steps taken is clearly less than k. If the walk starting at u restarts at v at step k before reaching x, it now needs to reach x from v, while restarting at v at every k steps. Let T be the steps taken to reach x from v. Let T' be the number of steps until the walk restarts at v, then exactly follows the shortest path from v to x for the first time, and then restarts at v. It is clear that $\mathbb{E}[T] \leq \mathbb{E}[T']$. Then, we split the walk of length T' into N trials, where each trial consists of restarting at v and walking k steps until the next restart. A trial is successful if it immediately walks the shortest path from v to x. Then N is the number of trials until we get a success, and it follows geometric distribution with probability of success at least $(1/\Delta)^{d(v,x)}$ only for $k \geq d(v, x)$, and zero for $k < d(v, x)$ since the walk cannot reach x before restart. Hence, its expectation is at most $\Delta^{d(v,x)}$ for $k \geq d(v, x)$, and we have $\mathbb{E}[T] \leq \mathbb{E}[T'] = k\mathbb{E}[N] \leq k\Delta^{d(v,x)}$. Adding the k steps until the first restart at v, we have:

$$H(u, x) \leq k + k\Delta^{d(v,x)}, \tag{74}$$

for any $k \geq d(v, x)$. Using $d(v, x) \leq r$, we get Equation 55. This completes the proof. □

We now extend Lemma A.4 to edges. Let $H(u, (x, y))$ be the expected number of steps of a random walk starting at u takes until traversing an edge (x, y) by $x \to y$. We show that $H(u, (x, y))$ is finite for any u and adjacent x, y in $B_r(v)$ for any nonzero restart probability α or restart period $k \geq r + 1$.

Lemma A.5. *For any u and adjacent x, y in $B_r(v)$, $H(u, (x, y))$ is bounded by the following:*

$$H(u, (x, y)) \leq \frac{1}{\alpha} + \frac{1}{\alpha}\left(\frac{\Delta}{1-\alpha}\right)^{r+1} + \frac{1}{\alpha}\left(\frac{1}{\alpha} - 1\right)\left(\frac{\Delta}{1-\alpha}\right)^{2r+1}, \tag{75}$$

if the random walk restarts at v with any probability $\alpha \in (0, 1)$, and:

$$H(u, (x, y)) \leq k + k\Delta^{r+1}, \tag{76}$$

if the random walk restarts at v with any period $k \geq r + 1$.

Proof. The proof is almost identical to Lemma A.4, except the target x of reaching is substituted by (x, y) in the direction of $x \to y$, and all arguments that use the shortest path from u or v to x instead use the shortest path to x postfixed by $x \to y$, which adds $+1$ to several terms in the bounds. □

We are now ready to prove Theorem 2.5.

Theorem 2.5. *In Theorem 2.4, if the random walk restarts at v with any nonzero probability α or any period $k \geq r + 1$, the vertex and edge cover times of $B_r(v)$ are always finite.*

Proof. The proof is inspired by the spanning tree argument of Aleliunas et al. (1979). Let us consider a depth first search of $B_r(v)$ starting from v. We denote by T the resulting spanning tree with vertices $V(T) = V(B_r(v))$. We consider the expected time for a random walk starting at v to visit every vertex in the precise order visited by the depth first search by traversing each edge twice. It is clear that this upper-bounds the vertex cover time of $B_r(v)$ starting at v (Equation 18):

$$C_V(B_r(v)) \leq \sum_{(x,y)\in E(T)} [H(x, y) + H(y, x)]. \tag{77}$$

Then, using the bounds from Lemma A.4, the property of spanning trees $|E(T)| = |V(T)| - 1$, and the fact that $|V(T)| = |V(B_r(v))| \leq \Delta^r$ from bounded degree, we obtain:

$$C_V(B_r(v)) \leq 2(\Delta^r - 1)\left(\frac{1}{\alpha} + \frac{1}{\alpha}\left(\frac{\Delta}{1-\alpha}\right)^{r} + \frac{1}{\alpha}\left(\frac{1}{\alpha} - 1\right)\left(\frac{\Delta}{1-\alpha}\right)^{2r}\right), \tag{78}$$

if the random walk restarts at v with any probability $\alpha \in (0, 1)$, and:

$$C_V(B_r(v)) \leq 2(\Delta^r - 1)(k + k\Delta^r), \tag{79}$$

if the random walk restarts at v with any period $k \geq r$. This completes the proof for the vertex cover time. For the edge cover time, we consider the expected time for a random walk starting at v to visit every edge in the precise order discovered[6] by the depth first search by traversing each edge twice. It is clear that this upper-bounds the edge cover time of $B_r(v)$ starting at v (Equation 19):

$$C_E(B_r(v)) \leq \sum_{(x,y)\in E(B_r(v))} [H(x,(x,y)) + H(y,(y,x))]. \tag{80}$$

Then, using Lemma A.4 and the fact that $|E(B_r(v))| \leq \Delta^{2r} - 1$ from bounded degree, we obtain:

$$C_E(B_r(v)) \leq 2(\Delta^{2r}-1)\left(\frac{1}{\alpha} + \frac{1}{\alpha}\left(\frac{\Delta}{1-\alpha}\right)^{r+1} + \frac{1}{\alpha}\left(\frac{1}{\alpha}-1\right)\left(\frac{\Delta}{1-\alpha}\right)^{2r+1}\right), \tag{81}$$

if the random walk restarts at v with any probability $\alpha \in (0,1)$, and:

$$C_E(B_r(v)) \leq 2(\Delta^{2r}-1)\cdot(k + k\Delta^{r+1}), \tag{82}$$

if the random walk restarts at v with any period $k \geq r+1$. This completes the proof. □

While our proof shows finite bounds for the cover times, it is possible that they can be made tighter, for instance based on Zuckerman (1991). We leave improving the bounds as a future work.

A.5.7 Proof of Theorem 3.2 (Section 3.1)

We recall universal approximation of graph-level functions in probability (Definition 3.1):

Definition 3.1. *We say $X_\theta(\cdot)$ is a universal approximator of graph-level functions in probability if, for all invariant functions $\phi : \mathbb{G}_n \to \mathbb{R}$ for a given $n \geq 1$, and $\forall \epsilon, \delta > 0$, there exist choices of length l of the random walk and network parameters θ such that the following holds:*

$$\mathrm{Prob}[|\phi(G) - X_\theta(G)| < \epsilon] > 1 - \delta, \quad \forall G \in \mathbb{G}_n. \tag{83}$$

We remark that an RWNN $X_\theta(\cdot)$ is composed of a random walk algorithm, a recording function $q : (v_0 \to \cdots \to v_l, G) \mapsto \mathbf{z}$, and a reader neural network $f_\theta : \mathbf{z} \mapsto \hat{\mathbf{y}} \in \mathbb{R}$.

Intuitively, if the record $\mathbf{z}$ of the random walk always provides complete information of the input graph G, we may invoke universal approximation of f_θ to always obtain $|\phi(G) - f_\theta(\mathbf{z})| < \epsilon$, and thus $|\phi(G) - X_\theta(G)| < \epsilon$. However, this is not always true as the random walk may e.g. fail to visit some vertices of G, in which case the record $\mathbf{z}$ would be incomplete. As we show below, this uncertainty leads to the probabilistic bound $> 1 - \delta$ of the approximation.

Let us denote the collection of all possible random walk records as $\{\mathbf{z}\} \coloneqq \mathrm{Range}(q)$, and consider a decoding function $\psi : \{\mathbf{z}\} \to \mathbb{G}_n$ that takes the record $\mathbf{z} \coloneqq q(v_0 \to \cdots \to v_l, G)$ of a given random walk $v_{[\cdot]}$ and outputs the graph $\psi(\mathbf{z}) \in \mathbb{G}_n$ composed of all recorded vertices $V(H) \coloneqq \{\mathrm{id}(v_t) : v_t \in \{v_0, ..., v_l\}\}$ and all recorded edges $E(H) \subset V(H) \times V(H)$. We show the following lemma:

Lemma A.6. *Let $G_\mathbf{z}$ be the subgraph of G whose vertices and edges are recorded by $\mathbf{z}$. Then the graph $\psi(\mathbf{z})$ decoded from the record $\mathbf{z}$ is isomorphic to $G_\mathbf{z}$ through the namespace $\mathrm{id}(\cdot)$:*

$$G_\mathbf{z} \overset{\mathrm{id}}{\simeq} \psi(\mathbf{z}). \tag{84}$$

Furthermore, the decoded graph $\psi(\mathbf{z})$ reconstructs G up to isomorphism, that is,

$$G \overset{\mathrm{id}}{\simeq} \psi(\mathbf{z}), \tag{85}$$

if the recording function $q(\cdot)$ and the random walk $v_{[\cdot]}$ satisfies either of the following:

- *$q(\cdot)$ uses anonymization, and $v_{[\cdot]}$ has traversed all edges of G.*
- *$q(\cdot)$ uses anonymization and named neighbors, and $v_{[\cdot]}$ has visited all vertices of G.*

[6] We remark that depth first search discovers all edges of a graph, while not necessarily visiting all of them.

Proof. Equation 84 is straightforward from the fact that the namespace $\mathrm{id}(\cdot)$ defines a bijection from $V(G_{\mathbf{z}})$ to $[|V(G_{\mathbf{z}})|]$, and the recording function uses names $\mathrm{id}(v_t)$ to record vertices and edges. Equation 85 is satisfied when all vertices and edges of G have been recorded, i.e. $G_{\mathbf{z}} = G$, which is possible either when the random walk has traversed all edges of G, or when it has traversed all vertices of G and named neighbors are used to record the induced subgraph $G[V(G)] = G$. □

We further remark Markov's inequality for any nonnegative random variable T and $a > 0$:

$$\mathrm{Prob}[T \geq a] \leq \frac{\mathbb{E}[T]}{a}. \tag{86}$$

We are now ready to prove Theorem 3.2.

Theorem 3.2. *An RWNN $X_\theta(\cdot)$ with a sufficiently powerful f_θ is a universal approximator of graph-level functions in probability (Definition 3.1) if it satisfies either of the below:*

- *It uses anonymization to record random walks of lengths $l > C_E(G)/\delta$.*
- *It uses anonymization and named neighbors to record walks of lengths $l > C_V(G)/\delta$.*

Proof. Instead of directly approximating the target function $\phi : \mathbb{G}_n \to \mathbb{R}$, it is convenient to define a proxy target function on random walk records $\phi' : \{\mathbf{z}\} \to \mathbb{R}$ where $\{\mathbf{z}\} \coloneqq \mathrm{Range}(q)$ as follows:

$$\phi' \coloneqq \phi \circ \psi, \tag{87}$$

where $\psi : \{\mathbf{z}\} \to \mathbb{G}_n$ is the decoding function of walk records. Then, for a given $\mathbf{z}$, we have:

$$G \simeq \psi(\mathbf{z}) \quad \Longrightarrow \quad \phi(G) = \phi'(\mathbf{z}), \tag{88}$$

which is because ϕ is an invariant function, so $\phi(G) = \phi(\psi(\mathbf{z})) = \phi \circ \psi(\mathbf{z}) = \phi'(\mathbf{z})$. Then we have:

$$\mathrm{Prob}[G \simeq \psi(\mathbf{z})] \leq \mathrm{Prob}[|\phi(G) - \phi'(\mathbf{z})| = 0]. \tag{89}$$

We now invoke universality of f_θ to approximate ϕ'. If f_θ is a universal approximator of functions on its domain $\{\mathbf{z}\} \coloneqq \mathrm{Range}(q)$, for any $\epsilon > 0$ there exists a choice of θ such that the below holds:

$$|\phi'(\mathbf{z}) - f_\theta(\mathbf{z})| < \epsilon, \quad \forall \mathbf{z} \in \mathrm{Range}(q). \tag{90}$$

Combining Equations 89 and 90, we have:

$$\mathrm{Prob}[G \simeq \psi(\mathbf{z})] \leq \mathrm{Prob}[|\phi(G) - \phi'(\mathbf{z})| + |\phi'(\mathbf{z}) - f_\theta(\mathbf{z})| < \epsilon]. \tag{91}$$

We remark triangle inequality of distances on $\mathbb{R}$, for a given $\mathbf{z}$:

$$|\phi(G) - f_\theta(\mathbf{z})| \leq |\phi(G) - \phi'(\mathbf{z})| + |\phi'(\mathbf{z}) - f_\theta(\mathbf{z})|, \tag{92}$$

which implies, for a given $\mathbf{z}$:

$$|\phi(G) - \phi'(\mathbf{z})| + |\phi'(\mathbf{z}) - f_\theta(\mathbf{z})| < \epsilon \quad \Longrightarrow \quad |\phi(G) - f_\theta(\mathbf{z})| < \epsilon, \tag{93}$$

and hence:

$$\mathrm{Prob}[|\phi(G) - \phi'(\mathbf{z})| + |\phi'(\mathbf{z}) - f_\theta(\mathbf{z})| < \epsilon] \leq \mathrm{Prob}[|\phi(G) - f_\theta(\mathbf{z})| < \epsilon]. \tag{94}$$

Combining Equations 91 and 94, we have:

$$\mathrm{Prob}[|\phi(G) - f_\theta(\mathbf{z})| < \epsilon] \geq \mathrm{Prob}[G \simeq \psi(\mathbf{z})], \tag{95}$$

which can be written as follows:

$$\mathrm{Prob}[|\phi(G) - X_\theta(G)| < \epsilon] \geq \mathrm{Prob}[G \simeq \psi(\mathbf{z})]. \tag{96}$$

We now consider the probability of the event $G \simeq \psi(\mathbf{z})$ based on Lemma A.6. We first consider the case where the recording function $q(\cdot)$ uses anonymization. In this case, $G \simeq \psi(\mathbf{z})$ is achieved if the random walk of length l has traversed all edges of G. Let $T_E(G, v_0)$ be the number of steps that a random walk starting at v_0 takes until traversing all edges of G. Since the edge cover time $C_E(G)$ is its expectation taken at the worst possible starting vertex (Equation 17), we have the following:

$$\mathbb{E}[T_E(G, v_0)] \leq C_E(G), \quad \forall v_0 \in V(G), \tag{97}$$

which leads to the following from Markov's inequality (Equation 86):

$$\text{Prob}[T_E(G, v_0) < l] \geq 1 - \frac{\mathbb{E}[T_E(G)]}{l} \geq 1 - \frac{C_E(G)}{l}. \tag{98}$$

For a given random walk $v_0 \to \cdots \to v_l$ and its record $\mathbf{z}$, the following holds:

$$T_E(G, v_0) < l \quad \Longrightarrow \quad G \simeq \psi(\mathbf{z}), \tag{99}$$

which implies the following:

$$\text{Prob}[T_E(G, v_0) < l] \leq \text{Prob}[G \simeq \psi(\mathbf{z})]. \tag{100}$$

Combining Equations 96, 98, and 100, we have:

$$\text{Prob}[|\phi(G) - X_\theta(G)| < \epsilon] \geq 1 - \frac{C_E(G)}{l}. \tag{101}$$

Therefore, for any $\delta > 0$, if we choose $l > C_E(G)/\delta$ we would have the following:

$$\text{Prob}[|\phi(G) - X_\theta(G)| < \epsilon] > 1 - \delta. \tag{102}$$

This completes the proof for anonymization. The proof is identical for the recording function that uses anonymization and named neighbors, except that the edge cover time is changed to the vertex cover time $C_V(G)$ (Equation 16). This is because neighborhood recording automatically records the induced subgraph of visited vertices, thus visiting all vertices implies recording all edges, $G[V(G)] = G$. □

A.5.8 Proof of Theorem 3.4 (Section 3.1)

Theorem 3.4. *An RWNN $X_\theta(\cdot)$ with a sufficiently powerful f_θ and any nonzero restart probability α or restart period $k \geq r + 1$ is a universal approximator of vertex-level functions in probability (Definition 3.3) if it satisfies either of the below for all $B_r(v) \in \mathbb{B}_r$:*

- *It uses anonymization to record random walks of lengths $l > C_E(B_r(v))/\delta$.*
- *It uses anonymization and named neighbors to record walks of lengths $l > C_V(B_r(v))/\delta$.*

Proof. The proof is almost identical to Theorem 3.2, except $G \in \mathbb{G}_n$ are substituted by $B_r(v) \in \mathbb{B}_r$, and the decoding function $\psi : \{\mathbf{z}\} \to \mathbb{B}_r$ is defined to ignore all recorded vertices $\text{id}(x)$ whose shortest path distance from the starting vertex $\text{id}(v) = \text{id}(v_0) = 1$ exceeds r. The latter is necessary to restrict the range of the decoding function ψ to $\mathbb{B}_r$. In addition, any nonzero restart probability α or restart period $k \geq r + 1$ is sufficient to make the cover times $C_E(B_r(v))$ and $C_V(B_r(v))$ finite (Theorem 2.5), thereby guaranteeing the existence of a finite choice of l. □

A.5.9 Proof of Theorem 3.5 (Section 3.2)

Theorem 3.5. *The simple RWNN outputs $\mathbf{h}^{(l)} \to \mathbf{x}^\top \boldsymbol{\pi}$ as $l \to \infty$.*

Proof. Since G is connected and non-bipartite, the uniform random walk on it defines an ergodic Markov chain with a unique stationary distribution $\boldsymbol{\pi}$. The limiting frequency of visits on each vertex v is precisely the stationary probability $\boldsymbol{\pi}_v$. Since the model reads $\mathbf{x}_{v_0} \to \cdots \to \mathbf{x}_{v_l}$ by average pooling, the output is given by weighted mean $\sum_v \boldsymbol{\pi}_v \mathbf{x}_v$ which is $\mathbf{x}^\top \boldsymbol{\pi}$. □

A.5.10 Proof of Theorem 3.6 (Section 3.2)

Theorem 3.6. *Let $\mathbf{h}_u^{(l)}$ be output of the simple RWNN queried with u. Then:*

$$\mathbb{E}\left[\left|\frac{\partial \mathbf{h}_u^{(l)}}{\partial \mathbf{x}_v}\right|\right] = \frac{1}{l+1}\left[\sum_{t=0}^{l} P^t\right]_{uv} \to \boldsymbol{\pi}_v \quad \textit{as} \quad l \to \infty. \tag{103}$$

Proof. Since the model reads $\mathbf{x}_{v_0} \to \cdots \to \mathbf{x}_{v_l}$ by average pooling, the feature Jacobian $|\partial \mathbf{h}_u^{(l)} / \partial \mathbf{x}_v|$ is given as number of visits to the vertex v in the random walk $v_0 \to \cdots \to v_l$ starting at $v_0 = u$, divided by length $l+1$. Let us denote the expected number of these visits by $J(u, v, l)$. Let $\mathbb{1}_{v_t=v}$ be the indicator function that equals 1 if $v_t = v$ and 0 otherwise. Then we can write $J(u, v, l)$ as:

$$\begin{aligned} J(u, v, l) &= \mathbb{E}\left[\sum_{t=0}^{l} \mathbb{1}_{v_t=v} | v_0 = u\right], \\ &= \sum_{t=0}^{l} \mathbb{E}[\mathbb{1}_{v_t=v} | v_0 = u]. \end{aligned} \tag{104}$$

We have used linearity of expectations for the second equality. $\mathbb{E}[\mathbb{1}_{v_t=v} | v_0 = u]$ is the probability of being at v at step t given that the walk started at u. This probability is precisely $[P^t]_{uv}$. Therefore:

$$J(u, v, l) = \sum_{t=0}^{l} \left[P^t\right]_{uv} = \left[\sum_{t=0}^{l} P^t\right]_{uv}, \tag{105}$$

which gives the equality in Equation 103. Furthermore, since G is connected and non-bipartite, the uniform random walk on it defines an ergodic Markov chain with a unique stationary distribution $\boldsymbol{\pi}$. The limiting frequency of visits on vertex v is precisely the stationary probability $\boldsymbol{\pi}_v$, which gives the convergence in Equation 103. This completes the proof. □

A.6 Extended Related Work

Anonymized random walks (Micali & Zhu, 2016) The initial work on anonymization by Micali & Zhu (2016) has stated an important result, that a sufficiently long anonymized walk starting from a vertex v encodes sufficient information to reconstruct the local subgraph $B_r(v)$ up to isomorphism. While the focus of Micali & Zhu (2016) was a probabilistic graph reconstruction algorithm that uses a set of independent anonymized walks and accesses the oracle set of all possible anonymized walks, we adopt the idea in a neural processing context to acquire universality in probability (Section 3.1). In addition, the invariance property of anonymization has rarely been noticed formally in the literature, which is our key motivation for using it, on top of being able to recover the whole graph (Section 2).

In-depth comparison with CRaWl (Tönshoff et al., 2023) Our approach is related to CRaWl in two key aspects: **(1)** identity and connectivity encodings of CRaWl contains analogous information to anonymization and neighborhood recording, respectively, and **(2)** CRaWl uses 1D CNNs as the reader NN. A key technical difference lies in the first part. The identity and connectivity encodings of CRaWl are defined within a fixed window size (denoted s in (Tönshoff et al., 2023)), which puts a locality constraint on the recorded information. Precisely, the encodings at step t can encode the information of the walk from step $t - s$ to t (precisely, its induced subgraph), referred to as a walklet. The window size s is a hyperparameter that controls the expressive power of CRaWl, and this dependency makes CRaWl non-universal (Section 3.2, (Tönshoff et al., 2023)). Our choice of anonymization and neighborhood recording are not under such a local constraint, and they encode the full information of a given walk globally. This property underlies our universality results in Section 3.1, which also naturally motivates our choice of universal reader NNs, e.g. a transformer language model, which were not explicitly considered in CRaWl.

Random walks on graphs Our work builds upon theory of random walks on graphs, i.e. Markov chains on discrete spaces. Their statistical properties such as hitting and mixing times have been well-studied (Aleliunas et al., 1979; Lovász, 1993; Coppersmith et al., 1996; Feige, 1995; Oliveira, 2012; Peres & Sousi, 2015), and our method (Section 2) is related to vertex cover time (Aleliunas et al., 1979; Kahn et al., 1989; Ding et al., 2011; Abdullah, 2012), edge cover time (Zuckerman, 1991; Bussian, 1996; Panotopoulou, 2013; Georgakopoulos & Winkler, 2014), and improving them, using local degree information (Ikeda et al., 2009; Abdullah et al., 2015; David & Feige, 2018), non-backtracking (Alon et al., 2007; Kempton, 2016; Arrigo et al., 2019; Fasino et al., 2021), or restarts in case of infinite graphs (Dumitriu et al., 2003; McNew, 2013; Janson & Peres, 2012). Our work is also inspired by graph algorithms based on random walks, such as anonymous observation (Micali & Zhu, 2016), sublinear algorithms (Dasgupta et al., 2014; Chiericetti et al., 2016; Ben-Hamou et al., 2018;

Bera & Seshadhri, 2020), and personalized PageRank for search (Page et al., 1999). While we adopt their techniques to make our walks and their records well-behaved, the difference is that we use a deep neural network to process the records and directly make predictions. Our method is also related to label propagation algorithms (Zhu & Ghahramani, 2002; Zhu, 2005; Grady, 2006) that perform transductive learning on graphs based on random walks, which we further discuss in Section 5.3.

Over-smoothing and over-squashing Prior work on over-smoothing and over-squashing of MPNNs (Barceló et al., 2020; Topping et al., 2022; Giovanni et al., 2023; Giraldo et al., 2023; Black et al., 2023; Nguyen et al., 2023; Park et al., 2023; Wu et al., 2023) often make use of structural properties of graphs, such as effective resistance (Doyle & Snell, 1984; Chandra et al., 1997), Laplacian eigen-spectrum (Lovász, 1993; Spielman, 2019), and discrete Ricci curvatures (Ollivier, 2009; Devriendt & Lambiotte, 2022). Interestingly, random walks and their statistical properties are often closely related to these properties, indicating some form of parallelism between MPNNs and RWNNs. This has motivated our analysis in Section 3.2, where we transfer the prior results on over-smoothing and over-squashing of MPNNs based on these properties into the results on our approach.

Language models for learning on graphs While not based on random walks, there have been prior attempts on applying language models for problems on graphs (Wang et al., 2023; Chen et al., 2023b; Zhao et al., 2023; Fatemi et al., 2023; Ye et al., 2024), often focusing on prompting methods on problems involving simulations of graph algorithms. We take a more principle-oriented approach based on invariance and expressive power, and thus demonstrate our approach mainly on the related tasks, e.g. graph separation. We believe extending our work to simulating graph algorithms requires a careful treatment (Weiss et al., 2021; Delétang et al., 2023; de Luca & Fountoulakis, 2024; Sanford et al., 2024) and plan to investigate it as future work.

A.7 Limitations and Future Work

Our current main limitation is the cost of performing training and inference if using language models, especially on long walks. We believe efficient fine-tuning with e.g. low-rank adaptation (Hu et al., 2022; Chen et al., 2023a) may help overcome the issue. A question for future work is whether we can train a language model on a large pseudocorpus of random walks (Klubicka et al., 2019; 2020) to build a foundation model for graphs which is language-compatible. We plan to investigate this direction in the future.