## **Expectation-Complete Graph Representations with Homomorphisms**

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## Abstract

We investigate novel random graph embeddings that can be computed in expected polynomial time and that are able to distinguish all nonisomorphic graphs in expectation. Previous graph embeddings have limited expressiveness and either cannot distinguish all graphs or cannot be computed efficiently for every graph. To be able to approximate arbitrary functions on graphs, we are interested in efficient alternatives that become arbitrarily expressive with increasing resources. Our approach is based on Lovász' characterisation of graph isomorphism through an infinite dimensional vector of homomorphism counts. Our empirical evaluation shows competitive results on several benchmark graph learning tasks.

#### 1. Introduction

We study novel efficient and expressive graph embeddings motivated by Lovász' characterisation of graph isomorphism through homomorphism counts. While most graph embeddings drop completeness-the ability to distinguish all pairs of non-isomorphic graphs-in favour of runtime, we devise efficient embeddings that retain completeness in expectation. The specific way in which we sample a fixed number of pattern graphs guarantees an expectationcomplete embedding in expected polynomial time. In this way, repeated sampling will eventually allow us to distinguish all pairs of non-isomorphic graphs, a property that no efficiently computable deterministic embedding can guarantee. In comparison, most recent graph neural networks are inherently limited by the expressiveness of some k-dimensional Weisfeiler-Leman isomorphism test (Morris et al., 2019; Xu et al., 2019).

Our approach to achieve an expectation-complete graph embedding is based on homomorphism counts. These are known to determine various properties of graphs important for learning, such as the degree sequence or the eigenspectrum (Hoang & Maehara, 2020). Furthermore, homomorphism counts are related to the Weisfeiler-Leman hierarchy (Dvořák, 2010; Dell et al., 2018), which is the standard measure for expressiveness on graphs (Morris et al., 2019). They also determine subgraph counts (Curticapean et al., 2017) and the distance induced by the homomophism counts is asymptotically equivalent to the *cut distance*, which Grohe (2020) and Klopp & Verzelen (2019) motivated as an appropriate graph similarity for graph learning tasks.

In Section 2 we introduce the required concepts. In Section 3 we discuss that general expectation-complete embeddings can eventually distinguish all pairs of nonisomorphic graphs (Lemma 3), which leads to a universal representation (Theorem 4). Then we propose our expectation-complete embedding based on sampling entries from the Lovász vector (Theorem 7) and bound the number of samples required to provably get as close as desired to the full Lovász vector (Theorem 8). In Section 4, we show how to compute our embedding efficiently in expected polynomial time (Theorem 14). In Section 5, we show how to combine our embedding with graph neural networks. Finally, we discuss related work in Section 6 and show competitive results on benchmark datasets in Section 7 before Section 8 concludes.

### 2. Background and Notation

We start by defining the required concepts and notation. A graph G = (V, E) consists of a set V = V(G) of vertices and a set  $E = E(G) \subseteq \{e \subseteq V \mid |e| = 2\}$  of edges. In this work we only consider undirected graphs. The size v(G) of a graph G is the number of its vertices and by  $\mathcal{G}_n$  we denote the set of all graphs with size at most  $n \in \mathbb{N}$ . In the following F and G denote graphs, where F represents a pattern graph and G a graph in our training set. A homomorphism  $\Phi : V(F) \to V(G)$  is a map that preserves edges, i.e.  $\{v, w\} \in E(F) \Rightarrow \{\Phi(v), \Phi(w)\} \in E(G)$ . Note that homomorphisms, unlike subgraph isomorphisms, allow non-injectivity: multiple vertices of F can be mapped to the same vertex of G, see Figure 1. Let  $\operatorname{hom}(F, G)$  de-

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Figure 1. Example homomorphism: mapping a 4-cycle to an edge.

note the number of homomorphisms from F to G and let  $\varphi_{\mathcal{G}}(G) = (\hom(F,G))_{F \in \mathcal{G}}$  denote the vector of homomorphism counts from each graph of a family of graphs  $\mathcal{G}$  to G. We define the shorthand  $\varphi_n(G) = \varphi_{\mathcal{G}_n}(G)$ . We also define the homomorphism density t(F,G) = $\hom(F,G)/v(G)^{v(F)}$ , corresponding to the probability that a mapping from V(F) to V(G) drawn uniformly at random is a homomorphism. Similarly to  $\varphi$ , we define  $\psi_{\mathcal{G}}(G) = t(\mathcal{G}, G) = (t(F, G))_{F \in \mathcal{G}}$  and  $\psi_n(G) = \psi_{\mathcal{G}_n}$ . An *isomorphism* between two graphs G and G' is a bijection  $I: V(G) \to V(G')$  such that  $\{v, w\} \in E(G)$  if and only if  $\{I(v), I(w)\} \in E(G')$ . If there is an isomorphism between G and G', we say they are *isomorphic* and denote it as  $G \simeq G'$ . We say that a probability distribution  $\mathcal{D}$  over a countable domain  $\mathcal{X}$  has *full support* if each  $x \in \mathcal{X}$  has nonzero probability  $\Pr_{X \sim \mathcal{D}}(X = x) > 0.$ 

#### 2.1. Complete Graph Embeddings

Classical graph kernel and recent (neural) graph representation methods perform learning on graphs by (potentially implicitly) embedding them into a real vector space  $\mathcal{H}$ . A graph embedding is a map  $\varphi : \mathcal{G} \to \mathcal{H}$  defined on a set of graphs  $\mathcal{G}$ . A graph embedding  $\varphi$  is called *permutationinvariant* if for all  $G \simeq G' \in \mathcal{G}$  it holds that  $\varphi(G) = \varphi(G')$ . All common graph kernels (Kriege et al., 2020) and standard message-passing neural networks (Xu et al., 2019) are permutation-invariant. Now we define *completeness*, which requires the opposite direction of the implication.

**Definition 1.** A permutation-invariant graph embedding  $\varphi : \mathcal{G} \to V$  is complete (on  $\mathcal{G}$ ) if  $\varphi(G) \neq \varphi(G')$  for all non-isomorphic  $G, G' \in \mathcal{G}$ .

Completeness is necessary if we want to be *universal*, that is, be able to approximate any permutation-invariant function  $f : \mathcal{G} \to \mathbb{R}$ . In particular we would not be able to approximate a function f with  $f(G) \neq f(G')$  for two nonisomorphic graphs G and G' with  $\varphi(G) = \varphi(G')$ .

Complete graph embeddings allow to determine whether two graphs are isomorphic, as  $G \simeq G'$  if and only if  $\varphi(G) = \varphi(G')$ . Deciding graph isomorphism is a classical problem in graph theory whose computational complexity is a major open problem (Babai, 2016). While the problem is in NP, neither a polynomial-time algorithm is known nor it is known whether the problem is NP-complete. Thus, we always face a trade-off between efficiency and expressiveness: complete graph embeddings are unlikely to be computable in polynomial time (Gärtner et al., 2003) and hence most graph representations drop completeness in favour of polynomial runtime.

If  $\mathcal{H}$  is a (real) Hilbert space with inner product  $\langle \cdot, \cdot \rangle \to \mathbb{R}$ , and not just a vector space, we can define a graph kernel  $k_{\varphi}(G, G') = \langle \varphi(G), \varphi(G') \rangle$  using any permutationinvariant graph embedding  $\varphi : \mathcal{G} \to \mathcal{H}$ . We call  $k_{\varphi}$  complete if  $\varphi$  is complete. Note that

$$k_{\varphi}(G,G) - 2k_{\varphi}(G,G') + k_{\varphi}(G',G') = \|\varphi(G) - \varphi(G')\|^{2}$$
(1)

which for a complete kernel is 0 if and only if  $G \simeq G'$ . Thus, evaluating a complete graph kernel is at least as hard as deciding graph isomorphism, even if  $\varphi$  is not known or computed explicitly (Gärtner et al., 2003).

In this work, we avoid the previously mentioned trade-off by using random graph embeddings than can be computed in expected polynomial time. While dropping completeness, this allows us to keep a slightly weaker yet still desirable property: *completeness in expectation*.

#### **3. Expectation-Complete Graph Embeddings**

In the remainder of this work we will consider *random* graph embeddings. These are graph embeddings  $\varphi_X :$  $\mathcal{G} \to \mathcal{H}$  that are parameterised by a random variable X. Algorithmically, we can think of  $\varphi_X(G)$  as first sampling a random variable  $X \sim \mathcal{D}$  from a distribution  $\mathcal{D}$  and then computing  $\varphi_X(G)$ . If the expectation  $\mathbb{E}_{X \sim \mathcal{D}}[\varphi_X(G)]$  is defined for all  $G \in \mathcal{G}$ , we can define a (deterministic) graph embedding  $\mathbb{E}_{X \sim \mathcal{D}}[\varphi_X(\cdot)] : \mathcal{G} \to \mathcal{H}$ . This leads us to the central notion of this paper.

**Definition 2.** A random graph embedding  $\varphi_X$  is expectation-complete if the graph embedding  $\mathbb{E}_X[\varphi_X(\cdot)]$ is complete. The corresponding kernel  $k_X(G,G') = \langle \varphi_X(G), \varphi_X(G') \rangle$  is expectation-complete if  $\varphi_X$  is expectation-complete.

Expectation-complete graph embeddings satisfy a useful property, which no non-complete deterministic graph embedding can satisfy: they eventually will be complete if we sample often enough.

**Lemma 3.** Let  $\varphi_X : \mathcal{G} \to \mathcal{H}$  be a expectation-complete graph embedding and  $G, G' \in \mathcal{G}$  which are not isomorphic. For any  $\delta > 0$ , there exists  $L \in \mathbb{N}$  such that for all  $\ell \ge L$ 

 $(\varphi_{X_1}(G),\ldots,\varphi_{X_\ell}(G)) \neq (\varphi_{X_1}(G'),\ldots,\varphi_{X_\ell}(G'))$ 

with probability  $1 - \delta$ , where  $X_1, \ldots, X_\ell \sim \mathcal{D}$  i.i.d.

*Proof.* Let *G*, *G'* be non-isomorphic graphs. Since *φ*<sub>X</sub> is expectation-complete, it must hold that  $\mathbb{E}[φ_X(G)] \neq \mathbb{E}[φ_X(G')]$ , which in particular means that there exists a set  $A_{G,G'}$  of outcomes of *X* with  $\Pr(X \in A_{G,G'}) = p_{G,G'} > 0$  such that for all  $a \in A_{G,G'}$  it holds that  $φ_a(G) \neq φ_a(G')$ . We need  $\Pr(\exists i \in \{1, ..., \ell\} : X_i \in A_{G,G'}) \ge 1-\delta$ , hence  $1 - (1 - p_{G,G'})^{\ell} \ge 1 - \delta$  must hold. Solving for  $\ell$  we see that  $\ell \ge L = \left\lceil \frac{\log(1/\delta)}{\log(\frac{1}{1-p_{G,G'}})} \right\rceil$  is sufficient to guarantee that there will be at least one  $X_i$  in *A* with probability at least  $1 - \delta$ , implying  $φ_{X_i}(G) \neq φ_{X_i}(G')$ . □

This leads to the following result, that sampling eventually yields universality.

**Theorem 4.** Let  $n \in \mathbb{N}$ ,  $\varphi_X : \mathcal{G}_n \to \mathbb{R}^d$  be a finitedimensional expectation-complete graph embedding and  $f : \mathcal{G}_n \to \mathbb{R}$  a permutation-invariant function. For any  $\varepsilon > 0$  and  $\delta > 0$  there exists an  $\ell \in \mathbb{N}$  and a multi-layerperceptron  $g : \mathbb{R}^{d\ell} \to \mathbb{R}$  such that

$$|f(G) - g(\varphi_{X_1}(G), \dots, \varphi_{X_\ell}(G))| < \varepsilon$$

for all  $G \in \mathcal{G}_n$  with probability at least  $1 - \delta$ , where  $X_1, \ldots, X_\ell \sim \mathcal{D}$  i.i.d.

*Proof.* Let  $N = |\mathcal{G}_n|$ ,  $\mathcal{G}_n = \{G_1, \ldots, G_N\}$  and  $f(G_i) = y_i$  for all *i*. As in the proof of *Lemma* 3 we know that for each pair  $G, G' \in \mathcal{G}$  of non-isomorphic graphs there exists an event  $A_{G,G'}$  with non-zero probability  $p_{G,G'}$  guaranteeing that  $\varphi_X(G) \neq \varphi_X(G')$ . Let  $p = \min_{G,G'} p_{G,G'} > 0$ . We have to satisfy this for all pairs of non-isomorphic graphs simultaneously. By applying a union bound on the complement (meaning at least one  $A_{G,G'}$  does not happen) and bounding each of these terms through Lemma 3, we see that

$$\ell \ge \frac{\log |\mathcal{G}_n| + \log(1/\delta)}{\log(\frac{1}{1-p})}$$

samples are sufficient to guarantee that the embedding  $\varphi_{\ell}(G) = (\varphi_{X_1}(G), \dots, \varphi_{X_{\ell}}(G))$  is complete with probability  $1 - \delta$ . Note that  $\log |\mathcal{G}_n| \le n^2$ , meaning that if we treat p and  $\delta$  as constants then  $\mathcal{O}(n^2)$  many samples suffice.

It remains to show that there is an MLP g which can approximate the points  $(\varphi_{\ell}(G_1), y_1), \ldots, (\varphi_{\ell}(G_N), y_N)$ . It is clear that there exists a multivariate polynomial exactly fitting all the points. Then we can apply universal function approximation to the bounded region spanned by the N points and approximate the polynomial.

#### 3.1. Expectation-Completeness Through Graph Homomorphisms

We now present one way to achieve expectationcompleteness. We use the classical result of Lovász (1967) that all homomorphism counts up to  $n = \max\{v(G), v(G')\}$  determine if G and G' are isomorphic.

**Theorem 5** (Lovász (1967)<sup>1</sup>). Two graphs  $G, G' \in \mathcal{G}_n$  are isomorphic if and only if  $\varphi_n(G) = \varphi_n(G')$ .

This provides a powerful graph embedding for learning tasks on graphs (Dell et al., 2018; Hoang & Maehara, 2020; Barceló et al., 2021). We can define a simple kernel on  $\mathcal{G}_n$  with the canonical inner product using  $\varphi_n$ .

**Definition 6** (Complete Lovász kernel). Let  $k_{\varphi_n}(G, G') = \langle \varphi_n(G), \varphi_n(G') \rangle$ .

Note that  $\varphi_n$  and  $k_{\varphi_n}$  are both complete on  $\mathcal{G}_n$ , and hence can be used to distinguish non-isomorphic graphs of size up to n. We can use the Lovász vector embedding  $\varphi_n$  to devise graph embeddings that are expectation-complete. For that let  $e_F \in \mathbb{R}^{\mathcal{G}_n}$  be the '*F*th' standard basis unit-vector of  $\mathbb{R}^{\mathcal{G}_n}$ . For a distribution  $\mathcal{D}$  with full support on  $\mathcal{G}_n$  define the graph embedding  $\varphi_F(G) = \hom(F, G)e_F$  with  $F \sim \mathcal{D}$ .

**Theorem 7.** For a distribution  $\mathcal{D}$  with full support on  $\mathcal{G}_n$ and  $F \sim \mathcal{D}$ , the random embedding  $\varphi_F(\cdot)$  and the corresponding kernel are expectation-complete on  $\mathcal{G}_n$ .

*Proof.* Let  $\varphi_F$  with  $F \sim \mathcal{D}$  be as stated and  $G \in \mathcal{G}_n$ . Then

$$g = \mathbb{E}_F[\varphi_F(G)] = \sum_{F' \in \mathcal{G}_n} \Pr(F = F') \hom(F', G)e_{F'}.$$

The vector g has the entries  $(g)_{F'} = \Pr(F = F') \hom(F', G)$ . Let G' be a graph that is nonisomorphic to G and let  $g' = \mathbb{E}_F[\varphi_F(G')]$  accordingly. By Theorem 5 we know that  $\varphi_n(G) \neq \varphi_n(G')$ . Thus, there is an F' such that  $\hom(F', G) \neq \hom(F', G')$ . By definition of  $\mathcal{D}$  we have that  $\Pr(F = F') > 0$  and hence  $\Pr(F = F') \hom(F', G) \neq \Pr(F = F') \hom(F', G')$ which implies  $g \neq g'$ . That shows that  $\mathbb{E}_F[\varphi_F(\cdot)]$  is complete and concludes the proof.  $\Box$ 

We now analyse how close we are to the actual Lovász kernel, if we sample  $\ell$  patterns  $\mathcal{F} = (F_1, \ldots, F_\ell)$  i.i.d. from  $\mathcal{D}$ . We consider  $\varphi_{\mathcal{F}} = \sum_{F \in \mathcal{F}} \varphi_F$  and the kernel  $k_{\mathcal{F}}(G, G') = \langle \varphi_{\mathcal{F}}(G), \varphi_{\mathcal{F}}(G') \rangle$ . While formally working in  $\mathbb{R}^{\mathcal{G}_n}$ , we can restrict the analysis (and practical computation) to  $\mathbb{R}^{\mathcal{F}}$ , ignoring dimensions that only contain zeros.

We apply standard techniques similar to Rahimi & Recht (2007), Kontorovich & Nadler (2009), Shervashidze et al. (2009), and Wu et al. (2019). For convenience we will perform the analysis using the homomorphism densities  $\psi_F$ . Let  $D \in \mathbb{R}^{\mathcal{G}_n \times \mathcal{G}_n}$  be a diagional matrix with  $D_{FF} = \Pr_{X \sim \mathcal{D}}(X = F)$  and let  $J_F \in \{0, 1\}^{\mathcal{G}_n \times \mathcal{G}_n}$  be a matrix that is 1 at the *FF*th position and 0 everywhere else. For

<sup>&</sup>lt;sup>1</sup>For a more recent proof see Theorem 5.29 and the comments below in Lovász (2012).

the expectation of the random kernel  $\langle \psi_F(G), \psi_F(G') \rangle$  it holds that

$$\mathbb{E}_{F \sim \mathcal{D}}[\langle \psi_F(G), \psi_F(G') \rangle] = \mathbb{E}_{F \sim \mathcal{D}}[\psi_{\mathcal{G}_n}^{\mathsf{T}}(G)J_F\psi_{\mathcal{G}_n}(G')]$$
$$= \langle \sqrt{D}\psi_{\mathcal{G}_n}(G), \sqrt{D}\psi_{\mathcal{G}_n}(G') \rangle$$
$$=: k_{\mathcal{D}}(G, G').$$

Note that  $k_{\mathcal{D}}(G, G')$  is still a complete kernel as the complete graph embedding  $\psi_{\mathcal{G}_n}$  is just scaled by  $\sqrt{D}$ , which is invertible as  $\mathcal{D}$  has full support. For a sample  $\mathcal{F}$  of  $\ell$  patterns we get the joint (averaged) embedding  $\psi_{\mathcal{F}}(G) = 1/\sqrt{\ell}(t(F_1, G), \dots, t(F_\ell, G))$  and get the corresponding (averaged) kernel

$$\tilde{k}_{\mathcal{F}}(G,G') = \langle \psi_{\mathcal{F}}(G), \psi_{\mathcal{F}}(G') \rangle = \frac{1}{\ell} \sum_{i=1}^{\ell} \psi_{F_i}(G) \psi_{F_i}(G')$$

Applying a Hoeffding bound we get

$$\Pr\left(\left|\tilde{k}_{\mathcal{F}}(G,G') - k_{\mathcal{D}}(G,G')\right| > \varepsilon\right) \le 2e^{-2\varepsilon^2\ell}.$$

Note that the previous bound holds for a fixed pair G and G'. We can apply it to each pair in the training sample to get the following result.

**Theorem 8.** Let  $\varepsilon, \delta \in (0, 1)$ ,  $\mathcal{D}$  be a distribution on  $\mathcal{G}_n$ with full support, and let  $S \subseteq \mathcal{G}_n$  be a finite set of graphs. If we sample  $\mathcal{F} = (F_1, \ldots, F_\ell) \sim \mathcal{D}^\ell$  i.i.d. with

$$\ell = \mathcal{O}\left(\frac{\log(|S|/\delta)}{\varepsilon^2}\right)$$

we can guarantee that

$$\max_{G,G'\in S} \left| \tilde{k}_{\mathcal{F}}(G,G') - k_{\mathcal{D}}(G,G') \right| < \varepsilon$$

with probability at least  $1 - \delta$ .

*Proof.* We have to show that

$$\Pr\left(\max_{G,G'\in S}\left|\tilde{k}_{\mathcal{F}}(G,G')-k_{\mathcal{D}}(G,G')\right|>\varepsilon\right)<\delta.$$

By a union bound it is sufficient if

$$\sum_{G,G' \in S} \Pr\left( \left| \tilde{k}_{\mathcal{F}}(G,G') - k_{\mathcal{D}}(G,G') \right| > \varepsilon \right) < \delta$$

and by applying Hoeffding bound to each term in the sum get  $|S|^2 2e^{-2\varepsilon^2 \ell} < \delta$ . Solving for  $\ell$  yields that  $\ell = \mathcal{O}\left(\frac{\log(|S|/\delta)}{\varepsilon^2}\right)$  is sufficient.  $\Box$ 

**Corollary 9.** Let  $\varepsilon, \delta \in (0, 1)$ ,  $\mathcal{D}$  be a distribution on  $\mathcal{G}_n$  with full support. If we sample  $\mathcal{F} = (F_1, \ldots, F_\ell) \sim \mathcal{D}^\ell$  *i.i.d.* with

$$\ell = \mathcal{O}\left(\frac{n^2 + \log(1/\delta)}{\varepsilon^2}\right)$$

we can guarantee that

$$\max_{G,G'\in\mathcal{G}_n} \left| \tilde{k}_{\mathcal{F}}(G,G') - k_{\mathcal{D}}(G,G') \right| < \varepsilon$$

with probability at least  $1 - \delta$ .

*Proof.* Apply Theorem 8 with  $S = \mathcal{G}_n$ . We upper bound the number of graphs with up to n vertices as  $|\mathcal{G}_n| \le 2^{(n^2)}$ .

Hence, we achieve a bound for all graphs in  $\mathcal{G}_n$  while sampling only  $\mathcal{O}(n^2)$  patterns.

While we stated the previously achieved bounds for kernels, we can easily transform them to bounds on the induced distances of the graph embeddings using Equation (1).

**Corollary 10.** Let  $\varepsilon, \delta \in (0, 1)$ ,  $\mathcal{D}$  be a distribution on  $\mathcal{G}_n$  with full support. If we sample  $\mathcal{F} = (F_1, \ldots, F_\ell) \sim \mathcal{D}^\ell$  *i.i.d.* with

$$\ell = \mathcal{O}\left(\frac{n^2 + \log(1/\delta)}{\varepsilon^2}\right)$$

we can guarantee that for all  $G, G' \in \mathcal{G}_n$  simultaneously

$$\left| \left\| \psi_{\mathcal{F}}(G) - \psi_{\mathcal{F}}(G') \right\|^2 - \left\| \sqrt{D} (\psi_n(G) - \psi_n(G')) \right\|^2 \right| < \varepsilon$$

with probability at least  $1 - \delta$ .

Thus, our results apply not only to kernel methods, but also to learning methods that use the graph embedding directly, such as multilayer perceptrons.

#### 3.2. Graphs with Unbounded Size

In this section, we generalise the previous results to the set of all finite graphs  $\mathcal{G}_{\infty}$ . Theorem 5 holds for  $G, G' \in \mathcal{G}_{\infty}$ and the mapping  $\varphi_{\infty}$  that maps each  $G \in \mathcal{G}_{\infty}$  to an infinitedimensional vector. The resulting vector space, however, is not a Hilbert space with the usual inner product. To see this, consider any graph G that has at least one edge. Then hom $(P_n, G) \ge 2$  for every path  $P_n$  of length  $n \in \mathbb{N}$ . Thus, the inner product  $\langle \varphi_{\infty}(G), \varphi_{\infty}(G) \rangle$  is not finite.

To define a kernel on  $\mathcal{G}_{\infty}$  without fixing a maximum size of graphs, i.e., restricting to  $\mathcal{G}_n$  for some  $n \in \mathbb{N}$ , we define the countable-dimensional vector  $\varphi_{\infty}^{\downarrow}(G) = \left(\hom_{v(G)}(F,G)\right)_{F \in \mathcal{G}_{\infty}}$  where

$$\hom_{v(G)}(F,G) = \begin{cases} \hom(F,G) & \text{if } v(F) \le v(G) ,\\ 0 & \text{if } v(F) > v(G) . \end{cases}$$

That is,  $\varphi_{\infty}^{\downarrow}(G)$  is the projection of  $\varphi_{\infty}(G)$  to the subspace that gives us the homomorphism counts for all graphs of *size at most of G*. Note that this is

a well-defined map of graphs to a subspace of the  $\ell^2$  space, i.e., sequences  $(x_i)_i$  over  $\mathbb{R}$  with  $\sum_i |x_i|^2 < \infty$ . Hence, the kernel given by the canonical inner product  $k_{\infty}^{\downarrow}(G,G') = \langle \varphi_{\infty}^{\downarrow}(G), \varphi_{\infty}^{\downarrow}(G') \rangle_{\ell^2}$  is finite and positive semi-definite. Note that we can rewrite  $k_{\infty}^{\downarrow}(G,G') = k_{\min}(G,G') = \langle \varphi_{n'}(G), \varphi_{n'}(G') \rangle$  where  $n' = \min\{v(G), v(G')\}$ . While the first hunch might be to count patterns up to  $\max\{v(G), v(G')\}$ , this is not necessary to guarantee completeness.

## **Lemma 11.** $k_{\min}$ is a complete kernel on $\mathcal{G}_{\infty}$ .

The proof can be found in Appendix A.

Given a sample of graphs S, we note that for  $n = \max_{G \in S} v(G)$  we only need to consider patterns up to size n.<sup>2</sup> As the number of graphs of a given size n is superexponential, it is impractical to compute all such counts. Hence, we propose to resort to sampling.

**Theorem 12.** Let  $\mathcal{D}$  be a distribution on  $\mathcal{G}_{\infty}$  with full support and  $G \in \mathcal{G}_{\infty}$ . Then  $\varphi_F^{\downarrow}(G) = \hom_{v(G)}(F,G)e_F$  with  $F \sim \mathcal{D}$  and the corresponding kernel are expectation-complete.

The proof can be found in Appendix A.

Note that  $k_{\min}$  has the following interesting practical property. If we train a kernel-based classifier on a sample  $S \subseteq \mathcal{G}_n$  and want to classify a graph with size larger than n we do not have to recompute the embeddings  $\varphi_{\infty}^{\downarrow}(G)$  for  $G \in S$  as the terms corresponding to patterns with size > n in the kernel are zero anyway.

## 4. Computing Embeddings in Expected Polynomial Time

An expectation-complete graph embedding should be efficiently computable to be practical, otherwise we could simply use deterministic complete embeddings. In this section, we describe our main result achieving polynomial runtime in expectation. The best known algorithm (Díaz et al., 2002) to exactly compute hom(F, G) takes time

$$\mathcal{O}(v(F)v(G)^{\mathrm{tw}(F)+1}) \tag{2}$$

where tw(F) is the *treewidth* of the pattern graph F. Thus, a straightforward sampling strategy to achieve polynomial runtime in expectation is to give decreasing probability mass to patterns with higher treewidth. Unfortunately, in the case of  $\mathcal{G}_{\infty}$ , this is not possible.

**Proposition 13.** There exists no distribution  $\mathcal{D}$  with full support on  $\mathcal{G}_{\infty}$  such that the expected runtime of Eq. (2) becomes polynomial in v(G) for all  $G \in \mathcal{G}_{\infty}$ .

The proof can be found in Appendix A.

To resolve this issue we have to take the size of the largest graph in our sample into account. For a given sample  $S \subseteq \mathcal{G}_n$  of graphs, where *n* is the maximum number of vertices in *S*, we can construct simple distributions achieving polynomial time in expectation.

**Theorem 14.** There exists a distribution  $\mathcal{D}$  with full support on  $\mathcal{G}_n$  such that computing the expectation-complete graph embedding  $\varphi_F^{\downarrow}(G)$  with  $F \sim \mathcal{D}$  takes polynomial time in v(G) in expectation for all  $G \in \mathcal{G}_n$ .

*Proof sketch.* We first draw a treewidth upper bound k from an appropriate distribution. For example, to satisfy a runtime of  $\mathcal{O}(v(G)^{d+1})$  in expectation for some constant  $d \in \mathbb{N}$ , a Poisson distribution with  $\lambda \leq \frac{1+d\log n}{n}$  is sufficient for any  $G \in \mathcal{G}_n$ . We have to ensure that each possible graph with treewidth up to k gets a nonzero probability of being drawn. For that we first draw a k-tree—a maximal graph of treewidth k—and then take a random subgraph of it. See Appendix A for the full proof.

We do not require that the patterns are sampled uniformly at random. It merely suffices that each pattern has a nonzero probability of being drawn. We get a similar result for our random Lovász embedding.

**Theorem 15.** There exists a distribution  $\mathcal{D}$  with full support on  $\mathcal{G}_n$  such that computing the expectation-complete graph embedding  $\varphi_F(G)$  with  $F \sim \mathcal{D}$  takes polynomial time in v(G) in expectation for all  $G \in \mathcal{G}_n$ .

The proof can be found in Appendix A.

Combining these results with Theorem 8, we see that for any fixed  $\delta$  and  $\varepsilon$  we need in total an expected polynomial runtime to construct the embedding  $\varphi_{\mathcal{F}}$  with  $\mathcal{F} = (F_1, \ldots, F_\ell)$  with  $F_i \sim \mathcal{D}$  for all  $i \in \{1, \ldots, \ell\}$  and  $\ell$  as in Theorem 8.

### **5. Practical Application**

So far, we have restricted our discussion to graphs without node attributes. However, many real world datasets have attributes on their vertices and edges.We now discuss how to apply our embedding and kernel in such contexts.

It is conceptually possible to devise sampling schemes and corresponding distributions  $\mathcal{D}$  over graphs with discrete vertex and edge labels. However, in practice this tends to result in unusable probabilities. For any pattern F, a single edge with labeled endpoints which are not connected in G results in hom(F, G) = 0. Hence, the resulting graph embeddings  $\varphi_{\mathcal{F}}$  become very sparse and practically uninformative.

We instead propose to consider labeled graphs as unlabeled for the purpose of homomorphism counting and suggest to

<sup>&</sup>lt;sup>2</sup>It is sufficient to go up to the size of the second largest graph.



*Figure 2.* Architecture of combining expectation-complete embeddings with MPNN representations for graph learning.

include attribute information by applying a message passing graph neural network (GNN). Combining any GNN graph level representation with our embedding for a fixed set of sampled patterns  $\mathcal{F}$  as shown in Figure 2 is straightforward and allows to make any GNN architecture more expressive. In particular the direct sum of  $\varphi_{\mathcal{F}}$  and the GNN representation is expectation-complete on attributefree graphs; a property that the GNN representation alone does not posses. Theorem 4 then implies that we can approximate any function on  $\mathcal{G}_n$  using a suitable MLP with high probability.

## 6. Discussion and Related Work

*k*-WL test The *k*-dimensional Weisfeiler-Leman (WL) test<sup>3</sup> (Cai et al., 1992) and the Lovász vector restricted to the set  $\mathcal{T}_k$  of graph patterns with treewidth up to *k* are equally expressive (Dvořák, 2010; Dell et al., 2018), that is, they distinguish the same non-isomorphic graphs. Puny et al. (2023) discuss this relationship in the context of invariant polynomials. We now propose a random graph embedding with expected polynomial runtime that matches the expressiveness of *k*-WL in expectation. The same holds for MPNNs and *k*-GNNs, as their expressiveness is bounded by *k*-WL (Xu et al., 2019; Morris et al., 2019). Let  $\mathcal{D}$  be a distribution with full support on  $\mathcal{T}_k$  and  $\varphi_F^{k-WL}(\cdot)$  be the resulting random graph embedding where  $F \sim \mathcal{D}$ .

**Theorem 16.** The graph embedding  $\varphi_F^{k-WL}(\cdot)$  has the same expressiveness as the k-WL test in expectation for any  $\mathcal{D}$  that has full support on  $\mathcal{T}_k$ . Furthermore, there is a specific such distribution  $\mathcal{D}$  such that we can compute  $\varphi_F^{k-WL}(G)$  in expected polynomial time  $\mathcal{O}(v(G)^{k+1})$  for all  $G \in \mathcal{G}_{\infty}$ .

Proposition 13 does not apply to the embedding  $\varphi_F^{k\text{-WL}}(\cdot)$ . In particular, the used distribution, which guarantees expected polynomial runtime, is independent of n and can be used for all  $\mathcal{G}_{\infty}$ .

As before, we can state Hoeffding-based bounds to approximate how close we are to the full embedding  $\varphi_{\mathcal{T}_k}$ . Morris et al. (2017) achieved similar bounds by sampling the *k*-tuple neighbourshoods of the *k*-WL test instead of the homomorphism counts.

Homomorphism-based graph embeddings. Dell et al. (2018) proposed a complete graph kernel based on homomorphism counts related to our  $k_{\min}$  kernel. Instead of implicitly restricting the embedding to only a finite number of patterns, as we do, they weigh the homomorphism counts such that the inner product defined on the whole Lovász vectors converges. However, Dell et al. (2018) do not discuss how to compute their kernel and so, our approach can be seen as an efficient sampling-based alternative to their theoretical weighted kernel.

Using graph homomorphism counts as a feature embedding for graph learning tasks was proposed by Hoang & Maehara (2020) and Kühner (2021). Hoang & Maehara (2020) discuss various aspects of homomorphism counts important for learning tasks, in particular, universality aspects and their power to capture certain properties of graphs, such as bipartiteness. Instead of relying on sampling patterns, which we use to guarantee expectation in completeness, they propose to use a small number of fixed pattern graphs. This limits the practical usage of their approach due to computational complexity reasons. In their experiments the authors only use tree (GHC-tree(6)) and cycle patterns (GHC-cycle(8)) up to size 6 and 8, respectively, whereas we allow patterns of arbitrary size and treewidth, guaranteeing polynomial runtime in expectation. Similarly to Hoang & Maehara (2020), we use the computed embeddings as features for a kernel SVM (with RBF kernel) and an MLP. For first results using an SVM, see our preliminary work at Welke et al. (2022) and Thiessen et al. (2022).

Instead of embedding the whole graph into a vector of homomorphism counts, Barceló et al. (2021) proposed to use rooted homomorphism counts as node features in conjunction with a graph neural network (GNN). They discuss the required patterns to be as or more expressive than the *k*-WL test. We achieve this in expectation when selecting an appropriate sampling distribution, as discussed above.

**Cut distance** The distance induced by the Lovász vector of all homomorphism counts is strongly related to the *cut distance* (Borgs et al., 2006; Lovász, 2012). The cut distance is a well-studied and important distance on graphs that captures global structural but also sampling-based local information. It is well known that the distance given by homomorphism counts is close to the cut

<sup>&</sup>lt;sup>3</sup>This refers to the *folklore k*-WL test, also called *k*-FWL.

distance and hence has similar favourable properties. The cut distance, and hence homomorphism counts, capture the behaviour of all permutation-invariant functions on graphs. Using Corollary 10 we see that this also holds for random embeddings, as they converge to the distance induced by the Lovász vector with high probability. For a discussion on the importance of the cut distance and homomorphism counts in the context of graph learning see Dell et al. (2018), Klopp & Verzelen (2019), Grohe (2020), and Hoang & Maehara (2020).

Random graph and node embeddings Wu et al. (2019) adapted random Fourier features (Rahimi & Recht, 2007) to graphs and proposed a sampling-based variant of the global alignment graph kernel. Similar samplingbased ideas were discussed before for the graphlet kernel (Shervashidze et al., 2009; Ghanem et al., 2021) and frequent-subtree kernels (Welke et al., 2015). The standard analysis of Rahimi & Recht (2007) does not apply in our situation, as they require a shift-invariant kernel. Also the analysis by Wu et al. (2019) does not apply here, as they use finite-dimensional node embeddings as a starting point. None of the previously mentioned papers discusses random graph features in the context of expressiveness or completeness. Fang et al. (2021) and Choromanski (2023) considered random features for node embeddings and node classification tasks.

**Random node initialisation** Instead of randomly embedding the whole graph, Abboud et al. (2021) and Sato et al. (2021) considered to initialise the vertices of the graphs with random labels. Through this they achieve universality in expectation. However, while for each realization of the random graph pattern F our graph embedding  $\varphi_F$  is universal in expectation and permutation-invariant, random node initialisation is only permutation-invariant in expectation.

Subgraph counts While subgraph counts are also a reasonable choice for expectation-complete graph embeddings, they have multiple drawbacks compared to homomorphism counts. Most importantly, from a computational perspective, computing subgraph counts even for graphs such as trees or paths is NP-hard (Alon et al., 1995; Marx & Pilipczuk, 2014), while we can compute homomorphism counts efficiently for pattern graphs with small treewidth (Díaz et al., 2002). In particular, all known exact algorithms for (induced) subgraph isomorphism counting have a worst-case runtime of  $\mathcal{O}(v(G)^{v(F)})$ , even for patterns with small treewidth. This one of the main reasons why the graphlet kernel (Shervashidze et al., 2009) and similar fixed pattern based approaches (Bouritsas et al., 2022) only count subgraphs up to size around 5 or are only sufficient. Alternative approaches exist, such as the cyclic pattern kernel (Horváth et al., 2004) and the neighbourhood-

Table 1. Performance of different GNNs on 9 OGB benchmarks and ZINC. Baseline of a GNN with homorphism counts is the same GNN without homomorphism counts. Results for GNNs with homorphism counts are averaged over 9 different random samples of pattern graphs.

	Top 1 / 2 / 3	Beats baseline
GIN	0%/0%/0%	-
GIN+hom	0% / 10% / 10%	100%
GCN	0%/0%/0%	-
GCN+hom	10% / 10% / 20%	90%
GIN+F	0% / 10% / 50%	-
GIN+hom +F	20% / 40% / 70%	90%
GCN+F	0% / 50% / 60%	-
GCN+hom+F	70% / 80% / 90%	90%

based kernel of Costa & De Grave (2010), that are efficiently computable in special cases, for example on most molecular graphs.

#### 7. Empirical Evaluation

We analyze the performance of our expectation-complete embedding that can be computed in expected polynomial time. The details of the pattern sampling process are described in Appendix A. We evaluate our proposed embeddings in two contexts. We investigate how graph embeddings from message passing graph neural network (GNN) perform when augmented with our embeddings. To complement these results, we investigate the empirical expressive power of our embeddings on synthetic benchmark datasets. The code to sample patterns and to compute representations<sup>4</sup>, as well as for the GNN experiments<sup>5</sup> is available.

#### 7.1. Improving GNNs with Graph-Level Homomorphism Counts

For graph-level prediction tasks, GNNs compute a graph embedding which is used by an MLP to make the final prediction. We propose to extend the learned graph embedding by concatenating it with a vector of homomorphism counts for a set of up to 50 sampled patterns  $\mathcal{F}$  (cf. Section 5). As this approach is independent of the GNN it can boost the expressiveness of any GNN. Furthermore, it is possible to extend already trained GNNs by these patterns by simply changing the width of the MLP and fine tuning. We denote GNNs boosted by homomorphism counts by "GNN+hom". We compare two settings: with ("GNN+F") and without ("GNN") node and edge features. We determine whether our approach reliably boosts the prediction

<sup>&</sup>lt;sup>4</sup>Representations: github.com/pwelke/homcount

<sup>&</sup>lt;sup>5</sup>GNN evaluation: github.com/ocatias/HomCountGNNs

accuracy of GNNs.

Models. We use GIN (Xu et al., 2019) and GCN (Kipf & Welling, 2017) as baseline GNNs. We compare the baselines against GIN+hom and GCN+hom. When using homomorphism counts, we first train the model without these counts and then finetune the entire model with the full homomorphism vector. We normalize the vector of homomorphism counts such that each entry has 0 mean and a standard deviation of 1 over the training set. We base our hyperparameters on Hu et al. (2020) and tune only the dropout rate (for all hyperparameters see Table A in Appendix A). For models without homomorphism counts, we train and evaluate a model 10 times for the best hyperparameters. For models with homomorphism counts, we first find the best hyperparameters for one sample of homomorphism counts. Then, we train and evaluate the model with these hyperparameters for 8 different samples of pattern graphs and thus different homomorphism counts. For each model, we report the test result in the corresponding epoch with the best validation metric (see Appendix A). We report the average and standard deviation of all test results for a given type of model.

Setup. We evaluate on the commonly used molecule datasets ZINC, ogbg-molhiv and ogbg-moltox21 (Hu et al., 2020). Furthermore, we also train on 7 additional small molecule datasets from Hu et al. (2020) (see Appendix A). For ZINC we use the same setup as Bodnar et al. (2021): we use a batch size of 128 and an initial learning rate of  $10^{-3}$  which we reduce by half every 20 epochs without an improvement of the validation performance. We stop training after either 500 epochs or after the learning rate is smaller than  $10^{-5}$ . To finetune on ZINC, we restart the training procedure with an initial learning rate of  $5 \cdot 10^{-4}$ . For datasets based on OGB, we train for 100 epochs with a batch size of 32 and a fixed learning rate of  $10^{-3}$  which corresponds to the initial learning rate on ZINC. To finetune, we train for 100 additional epochs with a learning rate of  $5 \cdot 10^{-4}$ . We perform an ablation study in Appendix A.

**Results.** We summarize the results of the experiments in Table 1. The center column shows how often the best parameter setting for a variant (e.g. GIN+hom+F) was among the top 1, top 2, or top 3 scoring models among the ten datasets. Recall, that this references the predictive performance on the test in the epoch with the best performance on the validation set. We can immediately see that including homomorphism information is helpful for predictive performance as the best performing model for *every* dataset uses homomorphism counts. For each model, the rightmost column reports if a GNN variant with homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphism counts beats its respective baseline GNN without added homomorphi

Table 2. Accuracy on synthetic data

Method	CSL	PAULUS25
GIN	$10.00\pm0.00$	$7.14\pm0.00$
GNTK	$10.00\pm0.00$	$7.14\pm0.00$
GHC-Tree	$10.00\pm0.00$	$7.14\pm0.00$
GHC-Cycle	$100.0\pm0.00$	$7.14\pm0.00$
WL	$10.00\pm0.00$	$7.14\pm0.00$
Ours	$37.67 \pm 9.11$	$100.0\pm0.00$

momorphism counts. We can see that models with homomorphism counts outperform the baseline in at least 90% of the datasets. This demonstrates that besides theoretical guarantees, homomorphism counts also reliably improve the practical prediction performance of GNNs. Detailed results for all datasets and an ablation study can be found in Appendix A.

#### 7.2. Expressiveness on Synthetic Datasets

We complement these results on real world graph datasets with an empirical analysis of our approach on synthetic benchmark datasets used to evaluate the expressiveness of graph learning approaches. On these benchmarks the labels encode isomorphism classes. Both datasets are balanced and have 10 (CSL) and 14 (PAULUS25) classes, respectively. We sample a fixed number  $\ell = 50$  of patterns and compute the sampled min kernel (resp. the corresponding embedding) as described in Section 3.2. Table 2 shows averaged accuracies of an SVM classifier trained on our feature sets on the datasets CSL (Murphy et al., 2019) and PAULUS25 (Hoang & Maehara, 2020)<sup>6</sup>. We follow the experimental design of Hoang & Maehara (2020) and compare to their published results. We also included GNTK (Du et al., 2019), GIN (Xu et al., 2019), and the WL-kernel (Shervashidze et al., 2011). Even with as little as 50 features, it is interesting to note that a SVM with RBF kernel and our features performs perfectly on the PAULUS25 dataset, i.e., it is able to decide isomorphism for the strongly regular graphs in this dataset. On the CSL dataset the min kernel performs better than all competitors except GHC-cycle, which was specifically designed for this dataset. The performance of the min kernel on this dataset increases monotonically for larger number of patterns, for instance to 48.8% for 200 patterns, see Appendix A.

## 8. Conclusion

In this work, we introduced the notion of expectationcomplete graph embeddings—random embeddings, which in expectation can distinguish any pair of non-isomorphic graphs. We studied their general properties and have shown

<sup>&</sup>lt;sup>6</sup>Originally from www.distanceregular.org/graphs/paulus25.html

that repeated sampling will eventually allow us to distinguish any fixed pair of non-isomorphic graphs, which results in a universal representation for graphs of bounded size. We proposed to sample the Lovász vector of homomorphism counts as one possibility to achieve expectationcompleteness and have shown favourable properties, such as bounds on the convergence of the random embedding to the full Lovász vector. Using a specific distribution which gives exponentially decreasing probability to patterns with large treewidth, we showed that computing our embedding takes polynomial time in expectation. We discussed that homomorphism counts of patterns with treewidth up to k can be seen as a sampling-based variant of the k-WL test with the same expressiveness in expectation and that homomorphism counts are strongly related to the cut-distance. Our empirical results have shown that homomorphism counts of sampled patterns (a) tend to increase the performance of MPNNs on a set of benchmark datasets and (b) allow to learn classifiers that distinguish non-isomorphic graphs where MPNNs and other baselines fail.

As future work, we will investigate approximate counts to make our implementation more efficient (Beaujean et al., 2021). It is unclear how this affects expressiveness, as we loose permutation-invariance. Similar to Abboud et al. (2021) we would still retain permutation-invariance in expectation. Going beyond expressiveness results, our goal is to further study graph similarities suitable for graph learning, such as the cut distance as proposed by Grohe (2020). Finally, instead of sampling patterns from a fixed distribution, a more promising variant is to adapt the sampling process in a sample-dependent manner. One could, for example, draw new patterns until each graph in the sample has a unique embedding (up to isomorphism) or at least until we are at least as expressive as 1-WL on the given sample. Alternatively, we could pre-compute frequent or interesting patterns as proposed by Schulz et al. (2018) and use them to adapt the distribution. Such approaches would use the power of randomisation to select an appropriate graph embedding in a data-driven manner, instead of relying on a finite set of fixed and pre-determined patterns like previous work (Barceló et al., 2021; Bouritsas et al., 2022).

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# A. Appendix

The appendix will be released shortly. In the meantime, please contact the corresponding authors if you require more details.