Graph Representation Learning Through Recoverability

Maxim Fishman
Technion, Habana Labs
smax041@campus.technion.ac.il

Chaim Baskin
Technion
chainbaskin@cs.technion.ac.il

Evgenii Zheltonozhskii
Technion

Almog David
Technion

Ron Banner
Technion

Avi Mendelson
Technion

Abstract

Self-supervised learning methods became a popular approach for graph representation learning because they do not rely on manual labels and offer better generalization. Contrastive methods based on mutual information maximization between augmented instances of the same object are widely used in self-supervised learning of representations. For graph-structured data, however, there are two obstacles to successfully utilizing these methods: the data augmentation strategy and training decoder for mutual information estimation between augmented representations of nodes, sub-graphs, or graphs. In this work, we propose a self-supervised graph representation learning algorithm, Graph Information Representation Learning (GIRL). GIRL does not require augmentations or a decoder for mutual information estimation. The algorithm is based on an alternative information metric, recoverability, which is tightly related to mutual information but is less complicated when estimating. Our self-supervised algorithm consistently outperforms existing state-of-the-art contrast-based self-supervised methods by a large margin on a variety of datasets. In addition, we show how the recoverability can be used in a supervised setting to alleviate the effect of over-smoothing/squashing in deeper graph neural networks. The code to reproduce our experiments is available at
https://github.com/Anonymous1252022/Recoverability.

1 Introduction

Over the last decade, deep learning allowed researchers to tackle multiple hard tasks, previously considered intractable. For example, convolutional neural networks (CNNs) have been successfully applied to computer vision problems such as image classification [26], object detection [53], and semantic segmentation [56]. Nevertheless, while CNNs can process pixels successfully, multiple other modalities, including 3D meshes [67], social networks [55], brain connections [60], relational databases [15], citation graphs [59], and sensor networks [10], require the processing of irregular data. As a result, researchers have been looking into ways to exploit deep learning methods, such as CNNs, in order to work with graph-structured data. Deep learning on graphs and, in particular, graph neural networks [GNNs, 20, 39, 58], based on message passing [19], i.e., iterative updating of a graph node representation based on information aggregated from its neighbors, have become a very popular tool for machine learning with graphs.

Even though GNNs show exceptional ability to learn graph-based data representations in supervised learning scenarios, heavy reliance on labels highlights several of its shortcomings, including the cost of the collection and annotation of manual labels and poor generalization when training data is scarce. Self-supervised learning provides a promising learning paradigm that reduces the dependence on manual labels, addressing the drawbacks of supervised learning.

Currently, the most successive self-supervised methods are mostly contrast-based [24, 64, 76]. The contrast-based methods used in graph self-supervised learning commonly utilize the concept of

*Equal contribution.

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Graph Representation Learning Through Recoverability

Figure 1: A probabilistic model of our graph self-supervised learning algorithm GIRL, where a recoverability loss ($\rho(\cdot|\cdot)$) minimization technique is applied on a single GNN layer $g_{\theta_k}$. GNN layer $g_{\theta_k}$ receives node features $H^{(k)}$ and direct neighboring node features $Z^{(k)}$ as input, and outputs node embedding $H^{(k+1)}$. During self-supervised loss $L_{ssl}$ minimization, random vector $H^{(k+1)}$ aggregates information from pair $(H^{(k)}, Z^{(k)})$.

mutual information (MI) and data augmentation techniques, maximizing the estimated MI between augmented instances of the same object, e.g., a node, graph or sub-graph. The encoder–decoder designs of contrast-based graph self-supervised learning methods are rather complex, requiring sophisticated augmentation strategies and decoder training for MI estimation.

The MI maximization technique is widely used in deep learning [40, 52, 64], but MI estimation is hard, especially for high-dimensional random vectors [49]. The main difficulty comes from estimation of the high-dimensional probability density function from given samples, since generally the number of samples requires scaling exponentially with the dimension. This is impractical for realistic deep learning applications, such as GNNs, where the representations are high dimensional. As a result, neural entropic estimators [8, 12] were developed for mitigation of this shortcoming; however, they involve a lot of additional parameters that must be trained appropriately.

In this work we propose another information metric, recoverability. We prove that recoverability loss minimization leads to MI maximization. In parallel, we propose an efficient and differentiable method of recoverability loss estimation using kernel regression [4], which does not require additional learnable parameters. As a result, recoverability loss minimization is less complicated than MI maximization. Second, we propose a novel algorithm for graph representation self-supervised learning, GIRL (Graph Information Representation Learning), depicted in Fig. 1, which is based on recoverability. GIRL does not require a decoder and minimizes recoverability loss instead of direct MI maximization. In GIRL, we do not use data augmentation since the recoverability loss is calculated between the input and output of each layer rather than between augmented instances of the same object. When presenting our experimental results, we demonstrate that GIRL significantly outperforms previous state-of-the-art contrast-based self-supervised algorithms.

Additionally, we show experimentally that recoverability loss minimization can be used to tackle problems in graph supervised learning. Minimization of recoverability loss between graph representations and the target, along with supervised loss, reduces the effect of over-smoothing/squashing. The latter phenomenon leads to undesirable reduction of both training and test accuracy along with extending the GNN depth [3, 41, 63].

We summarize our main contributions as follows:

- We present an alternative information metric, recoverability, and an efficient and differentiable method for its estimation. Moreover, we prove that recoverability loss minimization leads to mutual information maximization.
- We develop a self-supervised algorithm for graph representation learning, GIRL, based on recoverability, which is less complicated than contrast-based methods for graph self-supervised learning. We provide experimental results, demonstrating that GIRL significantly outperforms previous state-of-the-art contrast-based algorithms.
- We show that the effect of over-smoothing/squashing can be alleviated using recoverability-based regularization during training deeper graph neural networks in supervised fashion.
2 Related Work

**MI estimation and application to deep learning.** Mutual information is a measure of dependency between two random variables and is a cornerstone of information theory. The MI maximization principle is widely used in deep learning. Yet, MI estimation remains a difficult task, especially for high-dimensional random vectors. Kleinman et al. [40] addressed this issue by introducing a notion of usable information, based on MI, which is contained in the representation learned by a deep network.

MI maximization can be used to learn better graph representations both in supervised and self-supervised settings [6, 52, 62]. In many recent works, MI is estimated via MINE [8] or its improvement, MI-NEE [12], which involves a lot of additional parameters that must be learned for correct MI estimation. Other approaches for MI estimation utilize finding lower bounds using variational Bayesian methods [1, 2, 7, 9].

**Self-supervised learning in GNNs.** We refer the reader to Liu et al. [43] for a comprehensive survey of modern graph self-supervised learning techniques. Graph self-supervised learning methods can be roughly split into four categories: generation-based, auxiliary property-based, contrast-based and hybrid. The generation-based methods aim to reconstruct the input data, and can be divided into two sub-categories: feature generation that learns to reconstruct the feature information of graphs [33, 44, 50, 66] and structure generation that learns to reconstruct the topological structure information of graphs [23, 29, 37, 48, 75]. In auxiliary property-based methods, the auxiliary properties are extracted from graph freely, afterwards the decoder aims to predict the extracted properties [34, 36, 42, 51, 77]. Contrastive methods can be classified by augmentation techniques: node feature masking [28, 32, 33, 70, 76], node feature shuffling [47, 54, 64], edge modification [30, 72, 73, 75], graph diffusion [18, 25], and sub-graph sampling [31]. Finally, hybrid methods [13, 16, 35, 57, 65, 68, 74] combine one or more of aforementioned methods.

3 Method

In this section we provide basic notations used throughout this paper and define a probabilistic model of a single GNN layer along with a collection of random vectors involved in the information aggregation process. We use these definitions to present a novel metric of information, recoverability, show its tight relation to MI, and offer an efficient and differentiable way to estimate it. We conclude this section by providing applications of recoverability in graph representation learning for both supervised and self-supervised settings. In the self-supervised setting we develop a novel algorithm, GIRL, for graph representation learning, whereas in the supervised setting we show how to use recoverability for improving information aggregation from neighboring node features.

3.1 Basic Notations

In this paper we mainly focus on node-attributed graphs and node classification tasks, either as a main task or as a downstream task for evaluation of self-supervised learning. We now provide the necessary notations and definitions, partially taken from Liu et al. [43].

A node attributed graph is a tuple $G = (V, E, \{x_i\}_{i \in [n]})$, where $V = \{v_1, \ldots, v_n\}$ ($|V| = n$) is the set of nodes, $E \subseteq V \times V$ ($|E| = m$) is the set of edges, and $\{x_i\}_{i \in [n]}$ are node features, where $[n] = \{1, 2, \ldots, n\}$. The collection of direct neighboring nodes of $v_i$ is denoted as $N(v_i)$, and the collection of indices of neighboring nodes of $v_i$ is denoted as $\mathcal{N}(i)$.

The node classification task aims to predict the label $y_i \in \mathcal{Y}$ for each node $v_i \in V$, where $\mathcal{Y}$ is a finite label set. Typically, the encoder $f_\theta$, parameterized by $\theta$, is applied to the node features $\{x_i\}_{i \in [n]}$, and generates node representations (embeddings) $\{h_i\}_{i \in [n]}$. Thereafter, the decoder $p_\phi$ parameterized by $\phi$, takes $\{h_i\}_{i \in [n]}$ as its input and generates logits. Finally, the cross-entropy (CE) loss $L_{ce}$ is optimized. The formulation of node classification is defined as follows:

$$\theta^*, \phi^* = \arg\min_{\theta, \phi} \frac{1}{|\mathcal{V}|} \sum_{v_i \in \mathcal{V}} L_{ce}(p_\phi([f_\theta(G)]_{v_i}), y_i)$$

where $[\cdot]_{v_i}$ is a choice function that indexes the embedding of $v_i$ from the set $\{h_i\}_{i \in [n]}$. 

Graph Representation Learning Through Recoverability
We denote by $H_f$ we first apply GNN where $l$ vector $Z$ vectors containing information about the neighborhood at each layer. To this end, we define a random $Y$ good estimation of random variable $H$ possible that is relevant to random variable $Y$. In a supervised setting we would like to extract from attributed graph $G$, In the following we define a probabilistic model of the information aggregation process of a single decoder $p$, During evaluation, we leverage the trained graph encoder $f_\theta$ with the frozen parameters of encoder $\theta^*$:

$$\phi^* = \arg \min_{\phi} \frac{1}{|V|} \sum_{v_i \in V} \mathcal{L}_{ce}(p_\phi([f_{\theta^*}(G)]_{v_i}), y_i)$$

3.2 Probabilistic Model of a GNN Layer

In the following we define a probabilistic model of the information aggregation process of a single GNN layer $g_{\theta^*}$. Fig. 2 demonstrates a single intermediate GNN layer $g_{\theta^*}$, which receives node features $h_i^{(k)}$ and direct neighboring node features $\{h_j^{(k)}\}_{j \in \mathcal{N}(i)}$ as input, and outputs node embedding $h_i^{(k+1)}$.

For each $k \in [l]$, we assume that $\{h_i^{(k)}\}_{v_i \in V}$ are drawn i.i.d. from some underlying distribution $D^{(k)}$. We denote by $H^{(k)}$ a random vector distributed according to this distribution $D^{(k)}$. Thus, the node features $\{x_i\}_{i \in [n]}$ are distributed according to random vector $H^{(0)}$. In addition, we define random vectors containing information about the neighborhood at each layer. To this end, we define a random vector $Z^{(k)}$ as follows: we pick some node $v_i$ in the graph uniformly and then pick some neighboring node $v_j$ from $\mathcal{N}(v_i)$ uniformly. The feature vector of $v_j$ at layer $k$, $h_j^{(k)}$, is a sample from random vector $Z^{(k)}$. This way we encode a graph structure into the random vector $Z^{(k)}$. Finally, we define $Y$, a random variable according to which node labels $y_i \in \mathcal{Y}$ are distributed.

3.3 Recoverability-Based Aggregation

In a supervised setting we would like to extract from attributed graph $G$ as much information as possible that is relevant to random variable $Y$ and store it in the node representation random vector $H^{(k)}$ for each layer $k \in [l]$. As a result, it will be possible to train the decoder $p_\phi$ to produce a good estimation of random variable $Y$. In contrast, in self-supervised representation learning, our
goal is to learn some meaningful representation of the nodes without using any labels \( Y \). Without labels, we can not know beforehand which information should be preserved in the node embedding so that the downstream task (node classification) is successful. In this case, we prefer to keep as much information as possible in the extracted features, i.e., we want to transfer as much information as possible from pair \( (H^{(k)}, Z^{(k)}) \) to random vector \( H^{(k+1)} \) for each layer \( k \in [l] \) during self-supervised training.

One way to accomplish this is via MI maximization. For the supervised setting, we maximize MI between node representations \( H^{(k)} \) and random variable \( Y \) for each layer \( k \in [l] \). This term can be added as an additional term to the supervised loss. In the self-supervised setting, we maximize MI between \( (H^{(k)}, Z^{(k)}) \) and \( H^{(k+1)} \) for each layer \( k \in [l] \). This criterion can be used as self-supervised loss \( L_{ssl} \).

Nevertheless, the estimation of MI from samples is challenging, especially for high-dimensional random vectors. As noted above, we propose an alternative information metric, recoverability, which is tightly related to MI, but is less complicated for estimation, and does not involve additional learnable parameters.

### 3.3.1 Recoverability

Given two random vectors \( X \) and \( Y \), with values in \( \mathbb{R}^m \) and \( \mathbb{R}^n \), respectively, we say that \( Y \) is fully recoverable from \( X \) if there exists a continuous map \( f : \mathbb{R}^m \to \mathbb{R}^n \) such that \( f(X) = Y \). Such a relation between \( X \) and \( Y \), however, does not necessarily exist, meaning that we cannot fully recover \( Y \) from \( X \). Nevertheless, \( X \) may still contain some information from which we can partially recover \( Y \). To measure the amount of such information in \( X \), we define

\[
C_X = \{ f(X) \mid f : \mathbb{R}^m \to \mathbb{R}^n \text{ is continuous function} \},
\]

i.e., the collection of all random vectors that could be fully recovered from \( X \), and evaluate the distance between random vector \( Y \) and the set \( C_X \):

\[
\rho(Y|X) = \inf_{Z \in C_X} d(Y,Z)
\]

where \( d \) is some distance function between two random variables, e.g., a metric induced by the \( L_p \) norm, \( \mathbb{E}[|X|^p]^{1/p} \). We call this quantity \( \rho(Y|X) \) the recoverability loss.

The following theorem demonstrates why MI maximization can be can be accomplished by recoverability loss minimization.

**Theorem 1** Suppose we are given random vector \( Y \). Random vector \( X \), which minimizes recoverability loss \( \rho(Y|X) \), also maximizes MI \( I(X;Y) \).

We provide the proof of Theorem 1 in Appendix A.1.

In the following theorem we show how recoverability loss can be estimated using reproducing kernel Hilbert space (RKHS) embeddings [5] with the universal kernel [45]. This approach also known as kernel regression [4].

**Theorem 2** Let \( \hat{\rho}(y|x) \) be an estimator of \( \rho(Y|X) \) on a finite collection of samples \( (x, y) = \{(x_k, y_k)\}_{k \in [N]} \), where the \( L_p \)-norm is used for measuring the distance between two random vectors, when \( p \in [1, \infty) \). The empirical estimation of \( \rho(Y|X) \) is given by

\[
\hat{\rho}(y|x) = \frac{1}{n} \sum_{i \in [n]} \frac{1}{N^{1/p}} \left\| \left( I - \Pi \right)y^{(i)} \right\|_p,
\]

where \( y^{(i)} \) is the \( i \)-th element of \( \{y_k\}_{k \in [N]} \), and \( \Pi \) is an orthogonal projection onto \( \text{Im}(K) \) where

\[
K_{ij} = \exp \left( -\frac{||x_i - x_j||^2}{2\sigma^2} \right)
\]

is a Gram matrix.

We provide the proof of Theorem 2 in Appendix A.2 and experiments on synthetic data in Appendix B.
of the decoder $p_\phi$ is highly dependent on how much information regarding $Y$ is aggregated in random vector $H^{(l)}$ (the final embedding produced by $f_\psi$), i.e., the ability to learn a map from random vector $H^{(l)}$ to random variable $Y$, which we call the embedding quality. The embedding quality can be measured by recoverability loss $\rho(Y|H^{(l)})$: a lower recoverability loss indicates that the embedding quality is higher.

For instance, assume that we have two encoders $f_{\theta_1}$ and $f_{\theta_2}$, which produce two different random vectors $H_1^{(l)}$ and $H_2^{(l)}$, respectively, and the distance between $Y$ and $C_{H_1^{(l)}}$ is smaller than between $Y$ and $C_{H_2^{(l)}}$, meaning that $Y$ is less recoverable from $H_2^{(l)}$ than from $H_1^{(l)}$. In other words, encoder $f_{\theta_1}$ aggregated more information for recovering $Y$ than encoder $f_{\theta_2}$.

To aggregate more information in each consecutive layer $k \in [l]$, we propose to use recoverability loss $\rho(Y|H^{(k)})$ as an additional additive term for CE loss $L_{ce}$, as follows:

$$\theta^*, \phi^* = \arg \min_{\theta, \phi} \frac{1}{n} \sum_{i \in [n]} L_{ce}(p_\phi(h_i^{(k)}), y_i) + \lambda \sum_{k \in [l]} \hat{\rho}(y|h^{(k)})$$ (8)

where $y = \{y_i\}_{i \in [n]}$, $h^{(k)} = \{h_i^{(k)}\}_{i \in [n]}$, $h_i^{(k)} = [g_{\theta_1} \circ \cdots \circ g_{\theta_l}([x_i]_{i \in [n]})]_v$, and $\theta = \{\theta_1, \ldots, \theta_l\}$.

### 3.3.3 Graph Information Representation Learning

In the self-supervised setting we no longer have labels $Y$. Therefore, we do not know which information should be preserved in $H^{(k)}$ for each layer $k \in [l]$, to ensure that the downstream task is successful. Consequently, we propose to transfer as much information as possible from $(H^{(k)}, Z^{(k)})$ to $H^{(k+1)}$, for each $k \in [l]$.

Random vector $H^{(k+1)}$ contains all the information regarding random vectors $H^{(k)}$ and $Z^{(k)}$, if there exist continuous maps $f_1$ and $f_2$ such that $f_1(H^{(k+1)}) = H^{(k)}$ and $f_2(H^{(k+1)}) = Z^{(k)}$. In this case, we have $\rho(H^{(k)}|H^{(k+1)}) + \rho(Z^{(k)}|H^{(k+1)}) = 0$. We propose an algorithm named GIRL (Graph Information Representation Learning) for self-supervised graph representation learning, where we minimize the common recoverability loss $\rho(H^{(k)}|H^{(k+1)}) + \rho(Z^{(k)}|H^{(k+1)})$ for each layer $k \in [l]$ in GNN $f_\theta$. The self-supervised loss is formulated as:

$$\theta^* = \arg \min_{\theta} \sum_{k \in [l-1]} \left( \hat{\rho}(h^{(k)}|h^{(k+1)}) + \hat{\rho}(z^{(k)}|h^{(k+1)}) \right)$$ (9)

where $h^{(k)} = \{h_i^{(k)}\}_{i \in [n]}$, $z_i^{(k)}$ is a uniformly sampled vector from the set $\{h_j^{(k)} \mid j \in N(i)\}$, $h_i^{(k)} = \{h_i^{(k)}\}_{i \in [n]}$, $h_i^{(k)} = [g_{\theta_1} \circ \cdots \circ g_{\theta_l}([x_i]_{i \in [n]})]_v$, and $\theta = \{\theta_1, \ldots, \theta_l\}$. The algorithm is presented in Algorithm 1 and depicted in Fig. 1.

### Algorithm 1 GIRL – Graph Information Representation Learning

| Input: $G = (\mathcal{V}, \mathcal{E}, \{x_i\}_{i \in [n]})$, $f_\theta = g_{\theta_1} \circ \cdots \circ g_{\theta_l}$ |
| Output: $f_\theta$ |
| for batch $I \subseteq [n]$ do |
| for layer $k \in [l]$ do |
| $\{h_i^{(k)}\}_{i \in [n]} \leftarrow g_{\theta_k}(\{h_i^{(k-1)}\}_{i \in [n]})$ where $h_i^{(0)} = x_i$ for each $i \in [n]$ |
| for $i \in I$ do |
| $z_i \leftarrow h_i^{(k-1)}$, where $j$ is uniformly sampled from $N(i)$ |
| end for |
| $\hat{\rho}_k \leftarrow \hat{\rho}(\{h_i^{(k-1)}\}_{i \in [n]}|\{h_i^{(k)}\}_{i \in [n]}) + \hat{\rho}(\{z_i^{(k-1)}\}_{i \in [n]}|\{h_i^{(k)}\}_{i \in [n]}$ |
| end for |
| $L_{sasl} \leftarrow \sum_{k \in [l]} \hat{\rho}_k$ |
| apply SGD step to minimize $L_{sasl}$ |
| end for |
4 Experiments

We now present our experimental results, using our recoverability loss minimization technique for graph representation learning in both supervised and self-supervised settings. In self-supervised settings we compare our algorithm GIRL (Algorithm 1) with other contrast-based methods, and in the supervised settings we demonstrate that recoverability loss minimization leads to better aggregation of information. For all the experiments we used transductive datasets: Cora, Citeseer, Pubmed [69], DBLP [17], and Amazon-Photos [61], and inductive datasets: Reddit [22], Reddit2 [71], PPI [78], ogbn-arxiv and ogbn-products [27]. Details about the datasets can be found in Table 4. All experiments were executed on Nvidia RTX A6000 GPUs.

4.1 Graph Self-Supervised Learning

We empirically evaluate the quality of our method for self-supervised graph representation learning, GIRL, on a variety of node classification tasks (transductive as well as inductive), and compare our results against those achieved by existing self-supervised methods: DGI [64], GRACE [76] and BGCL [24].

4.1.1 Experimental setup

All datasets that were not formally divided into training/test sets, were split randomly using a 80/20 ratio. We used a cluster data loader [14] for loading inductive datasets Reddit, Reddit2, PPI, ogbn-arxiv and ogbn-products whereas all transductive datasets, Cora, Citeseer, Pubmed, DBLP, and Amazon-Photos, were loaded as whole graphs. We used unsupervised representation learning (URL) [43] setting, i.e., applied Algorithm 1 on a simple GNN encoder $f_{\theta}$ with GCN [39] layers to obtain $\theta^*$, and evaluated the quality of the learned encoder $f_{\theta^*}$ by training decoder $p_{\phi}$ as described in Section 3.1.

4.1.2 Results

The results, averaged on ten training runs with different seeds, are summarized in Table 1. Our self-supervised method significantly surpasses previous self-supervised methods. GIRL is able to learn informative representations both for small- and large-scale graphs, while other methods often fail on large-scale graphs. We believe that the inductive nature of the chosen large graphs is the reason for other methods failure. It is known that learning on inductive graphs is harder compared to learning on transductive graphs [22]. Existing self-supervised methods do not provide results for Reddit2, ogbn-arxiv, and ogbn-products datasets. For comparison, we produced such results (marked with a *) on GRACE with the same model as used on GIRL. We observe how our algorithm improved the results using each of these three datasets.

4.2 Graph Supervised Learning

We now turn to the depth problem in GNNs caused by over-smoothing/squashing phenomena [3, 41, 63], and show that accuracy can be improved via auxiliary recoverability loss, as described in Eq. (8).

4.2.1 Experimental setup

To reproduce over-smoothing/squashing phenomena, we chose to train GNN model with different depths. The GNN model consists of two consecutive blocks, encoder $f_{\theta}$ and decoder $p_{\phi}$. The encoder $f_{\theta}$ has $l \in \{3, 6, 9, 12, 15, 18\}$ SAGE[21] layers. The decoder $p_{\phi}$ comprises three fully connected layers. Each layer in the model except for the last one is followed by ReLU activation and dropout with drop probability $0.1$. For all datasets (Reddit, Reddit2, ogbn-arxiv, ogbn-products and PPI), a cluster data loader [14] was used.

4.2.2 Results

The results are summarized in Table 2 and Fig. 3. First of all, it can be seen from Fig. 3, that along with depth extension, both training and test accuracy decrease, while the generalization gap does not increase. We conclude that the overfitting effect does not increase significantly with additional layers. Instead, we observe an over-smoothing/squashing phenomenon [3, 41, 63]. Table 2 demonstrates
Table 1: Summary of the results in terms of classification accuracy for the transductive datasets or the micro-F1 score for the inductive datasets, with standard deviation. All results are averaged on ten training runs with different seeds; the best results are highlighted in bold. Results that we reproduced using GRACE using the same model as used with GIRL are marked with a *.

| Dataset           | DGI | GRACE | BGCL | GIRL (ours) |
|-------------------|-----|-------|------|-------------|
| Cora              | 82.3 ± 0.6 | 84.0 ± 0.1 | 83.8 ± 0.3 | **88.3 ± 0.1** |
| Citeseer          | 71.8 ± 0.7 | 72.1 ± 0.5 | 72.7 ± 0.3 | **79.1 ± 0.3** |
| Pubmed            | 76.8 ± 0.6 | 86.7 ± 0.1 | - | **89.0 ± 0.0** |
| DBLP              | - | 84.2 ± 0.1 | - | **85.9 ± 0.1** |
| Amazon-Photos     | - | 92.2 ± 0.2 | 92.5 ± 0.2 | **95.6 ± 0.1** |

Table 2: The performance of the model with different depths along with or without weight decay (W.D.) and recoverability loss (Rec.). The table is separated into the three blocks according to depth, where the best results are highlighted in bold.

| Depth | W.D. | Rec. (ours) | Accuracy          |
|-------|------|-------------|--------------------|
|       |      |             | Reddit Reddit2 ogbn-arxiv ogbn-products PPI |
| 3     | -    | -           | **92.9 ± 0.1** 93.0 ± 0.1 66.2 ± 0.3 75.5 ± 0.3 86.6 ± 0.1 |
| 3     | ✓    | -           | **92.9 ± 0.1** 92.9 ± 0.1 65.9 ± 0.3 75.6 ± 0.3 85.9 ± 0.1 |
| 3     | -    | ✓           | **93.0 ± 0.1** 93.1 ± 0.1 66.2 ± 0.4 75.6 ± 0.2 86.8 ± 0.1 |
| 9     | -    | -           | 91.9 ± 0.2 90.3 ± 0.6 66.4 ± 0.5 75.8 ± 0.3 83.9 ± 0.1 |
| 9     | ✓    | -           | 91.5 ± 0.3 89.7 ± 1.1 65.3 ± 0.4 75.3 ± 0.5 82.2 ± 0.2 |
| 9     | -    | ✓           | **92.6 ± 0.1** 92.1 ± 0.1 67.2 ± 0.3 75.8 ± 0.1 85.0 ± 0.1 |
| 18    | -    | -           | 89.2 ± 0.3 33.3 ± 25.7 64.7 ± 0.2 73.2 ± 0.3 76.9 ± 1.5 |
| 18    | ✓    | -           | 88.4 ± 0.2 14.9 ± 0.0 63.4 ± 0.2 72.4 ± 0.9 74.3 ± 0.1 |
| 18    | -    | ✓           | **91.4 ± 0.4** 76.4 ± 1.0 65.7 ± 0.3 74.6 ± 0.4 80.2 ± 0.2 |

Table 4.3 Ablation Study

We now compare the performance of graph representations learned via GIRL (Algorithm 1), against the graph representations generated by a randomly initialized network, in the downstream task. We make the comparison on different GNN architectures as well on different numbers of layers. The encoder $f_\theta$ is composed of $k \in \{1, 2, 3, 4, 5\}$ GNN layers of one of the following types: GCNConv [39], GATv2Conv [11], GraphConv [46], and SAGEConv [21]. Each GNN layer is followed by ELU activation. The decoder $p_\phi$, used in the downstream task, consists of two fully connected layers with ELU activation between them. In the self-supervised setting, the encoder $f_\theta$ was first learned using Algorithm 1, then decoder $p_\phi$ was trained on frozen features $\theta^*$ (Section 3.1). In the setting with
Graph Representation Learning Through Recoverability

Figure 3: The drop in both training and test accuracy along with the GNN depth extension.

Figure 4: Comparison of test accuracy in the downstream tasks of the self-supervised setup and random initial setup, where in the random initial setup, the self-supervised training was skipped. Each column refers to a different dataset. Each row corresponds to a different GNN layer type.

In this paper we introduced a novel information metric, recoverability, and proved that recoverability loss minimization leads to MI maximization. By virtue of RKHS embedding with a universal kernel, estimation of recoverability loss is efficient and does not require additional learnable parameters. Hence, recoverability loss minimization becomes less challenging than MI maximization, especially for high-dimensional samples. Second, we developed a novel self-supervised graph representation learning algorithm, GIRL. GIRL is based on recoverability and requires neither a decoder for MI estimation nor data augmentation techniques, resulting in lower complexity compared to the existing graph self-supervised contrast-based methods. We demonstrate empirically that GIRL outperforms existing art, especially on large-scale graphs. Finally, in a supervised setting we use recoverability as

5 Conclusion

In this paper we introduced a novel information metric, recoverability, and proved that recoverability loss minimization leads to MI maximization. By virtue of RKHS embedding with a universal kernel, estimation of recoverability loss is efficient and does not require additional learnable parameters. Hence, recoverability loss minimization becomes less challenging than MI maximization, especially for high-dimensional samples. Second, we developed a novel self-supervised graph representation learning algorithm, GIRL. GIRL is based on recoverability and requires neither a decoder for MI estimation nor data augmentation techniques, resulting in lower complexity compared to the existing graph self-supervised contrast-based methods. We demonstrate empirically that GIRL outperforms existing art, especially on large-scale graphs. Finally, in a supervised setting we use recoverability as
an auxiliary loss, enforcing better representation learning at each GNN layer. Empirical results reveal that in deeper networks, where over-smoothing/squashing phenomenon presents, the recoverability loss optimization leads to better test accuracy, even when weight decay regularization fails.
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A Proofs

A.1 Proof of Theorem 1

We prove this theorem through $\sigma$-algebras, the objects taken from measure theory. A $\sigma$-algebra $\mathcal{A}$ is a collection of subsets of $\Omega$ where the following set of properties is satisfied:

1. $\emptyset \in \mathcal{A}$
2. $A \in \mathcal{A} \implies A^c \in \mathcal{A}$
3. $\{A_n\}_{n \in \mathbb{N}} \subseteq \mathcal{A} \implies \bigcup_{n \in \mathbb{N}} A_n \in \mathcal{A}$

Each random vector $X : \Omega \rightarrow \mathbb{R}^m$ has its own $\sigma$-algebra, which is defined as follows:

$$\sigma_X = \{X^{-1}(A) : A \in \mathcal{B}(\mathbb{R}^m)\} \quad (10)$$

where $\mathcal{B}(\mathbb{R}^m)$ is a Borel $\sigma$-algebra on $\mathbb{R}^m$, i.e., generated from topology on $\mathbb{R}^m$.

Minimization of recoverability loss $ho(Y|X) = \inf_{Z \in \mathcal{C}_X} d(Y,Z)$ by altering $X$ changes the set $\mathcal{C}_X$. When $\rho(Y|X) = 0$, $Y$ is in $\mathcal{C}_X$ and thus continuous map $f : \mathbb{R}^m \rightarrow \mathbb{R}^n$ exists, such that $f(X) = Y$.

This leads to the following relation between $\sigma$-algebras of $X$ and $Y$:

$$\sigma_Y \subseteq \sigma_X \quad (11)$$

On other hand, the conventional definition of the entropy of random vector $X$ is given by expectation of a negative logarithm of probability density function:

$$H(X) = E[-\ln f_X(X)] \quad (12)$$

The equivalent, measure theoretic definition of entropy $H(X)$ is given by:

$$H(\sigma_X) = \sup_{P \subseteq \sigma_X} \sum_{A \in P} -P(A) \ln P(A) \quad (13)$$

where $P$ is a $P$-almost partition of $\Omega$, i.e., satisfies the following:

1. $P(\cup_{A \in P} A) = 1$
2. $\forall A, B \in P \quad P(A \cap B) = 0$

From above definition we can conclude that the entropy is fully dependent only on a $\sigma$-algebra of a given random vector $X$, and whenever we have the inclusion $\sigma_Y \subseteq \sigma_X$, the entropy of $Y$ is less than or equal to the entropy of $X$, i.e., $H(\sigma_Y) \leq H(\sigma_X)$.

The mutual information (MI) between two random vectors $X$ and $Y$ is defined as:

$$I(X;Y) = H(X) + H(Y) - H(X,Y) = H(\sigma_X) + H(\sigma_Y) - H(\sigma_X \cup \sigma_Y) \quad (14)$$

When we apply condition Eq. (11) to Eq. (14), we receive:

$$I(X;Y) = H(Y), \quad (15)$$

which is the maximal MI that we can achieve by altering only random vector $X$. 

16
A.2 Proof of Theorem 2

Let $U \subset \mathbb{R}^m$ be a compact\(^2\) set,
\[
C(U) = \{ f : U \to \mathbb{R} \mid f \text{ is continuous function} \},
\]
and
\[
\forall x_1, x_2 \in U \quad k(x_1, x_2) = \exp \left( -\frac{\|x_1 - x_2\|^2}{2\sigma^2} \right).
\]

For each $x \in U$, define continuous function $k(x, \cdot) = \phi_x(\cdot)$, and construct the following functional space:
\[
\mathcal{H}_0 = \text{span}\{ \phi_x(\cdot) \mid \forall x \in U \}
\]
Define an inner product on $\mathcal{H}_0$ as follows:
\[
\left\langle \sum_{i=1}^{n} a_i \phi_{x_i}(\cdot), \sum_{j=1}^{m} b_j \phi_{x_j}(\cdot) \right\rangle = \sum_{i=1}^{n} \sum_{j=1}^{m} a_i b_j k(x_i, x_j)
\]
Let $\mathcal{H}$ be the completion of $\mathcal{H}_0$ with respect to this inner product. Now $\mathcal{H}$ is a reproducing kernel Hilbert space (RKHS) built from the kernel $k(\cdot, \cdot)$.

Since $k(\cdot, \cdot)$ is a universal kernel \([45]\), the set $\mathcal{H}$ is dense in $C(U)$ with respect to the supremum norm, i.e.:
\[
\forall f \in C(U) \quad \forall \epsilon > 0 \quad \exists g \in \mathcal{H} \text{ s.t. } \sup_{x \in U} |f(x) - g(x)| < \epsilon
\]
In addition, $\mathcal{H}$ has reproducing property:
\[
\forall f \in \mathcal{H} \quad \forall x \in U \quad f(x) = \langle f, \phi_x(\cdot) \rangle
\]
and thus we have:
\[
\rho(Y(i)|X) = \inf_{Z \in C_X} d(Y(i, Z)) = \inf_{f \in C(U)} d(Y(i), f(X)) = \inf_{f \in \mathcal{H}} d(Y(i), f(X)) = \inf_{f \in \mathcal{H}} d(Y(i), \langle f, \phi_X(\cdot) \rangle)
\]
We denote the estimation of $\rho(Y|X)$ on a finite collection of samples $(x, y) = \{(x_k, y_k)\}_{k \in [N]}$ by $\hat{\rho}(y|x)$ and use the distance induced from the $L_p$-norm, where $p \in [1, \infty)$. Thus we have:
\[
\hat{\rho}(y(i)|x) = \inf_{f \in \mathcal{H}} \left( \frac{1}{N} \sum_{k \in [N]} |y_k^{(i)} - \langle f, \phi_{x_k}(\cdot) \rangle|^p \right)^{1/p}
\]
From the representor theorem \([38]\), there exists $f^* \in \mathcal{H}$ of the following form:
\[
f^* = \sum_{i \in [N]} \alpha_i \phi_{x_i}(\cdot)
\]
which minimizes $\hat{\rho}(y(i)|x)$. Thus:
\[
\hat{\rho}(y(i)|x) = \left( \frac{1}{N} \sum_{k \in [N]} |y_k^{(i)} - \langle f^*, \phi_{x_k}(\cdot) \rangle|^p \right)^{1/p}
\]
\[
= \min_{\alpha \in \mathbb{R}^N} \left( \frac{1}{N} \sum_{k \in [N]} |y_k^{(i)} - \sum_{j \in [N]} \alpha_j k(x_j, x_k)|^p \right)^{1/p} = \min_{\alpha \in \mathbb{R}^N} \frac{1}{N^{1/p}} \|y^{(i)} - K \alpha\|_p
\]
\(^2\)It is not a restrictive assumption that $U$ is a compact set since all tensor values in neural networks are bounded.
where $K_{ij} = k(x_i, x_j)$ is a Gram matrix.

Decompose $y^{(i)}$ into two parts:

$$y^{(i)} = y^{(i)}_\parallel + y^{(i)}_\perp$$

(28)

where $y^{(i)}_\parallel \in \text{Im}(K)$ and $\forall v \in \text{Im}(K)$, $(y^{(i)}_\perp)^T v = 0$. Then we have:

$$\hat{\rho}(y^{(i)} | x) = \frac{1}{N^{1/p}} \left\| y^{(i)}_\parallel \right\|_p$$

(29)

Since $K$ is positive semi-definite, we have the following eigendecomposition:

$$K = U \Lambda U^T$$

(30)

where columns of unitary matrix $U$ are eigenvectors of $K$ and $\Lambda$ is a diagonal matrix of eigenvalues. Let:

$$\lambda_1, \lambda_2, ..., \lambda_k, 0, 0, ..., 0$$

(31)

be the descending order of eigenvalues, where $\lambda_k > 0$. Then,

$$\Pi = \sum_{i \in [k]} u_i u_i^T$$

(32)

is an orthogonal projection into $\text{Im}(K)$ subspace. Consequently,

$$\hat{\rho}(y^{(i)} | x) = \frac{1}{N^{1/p}} \left\| (I - \Pi)y^{(i)} \right\|_p$$

(33)

where $I$ is an identity matrix. And thus, we have:

$$\hat{\rho}(y | x) = \frac{1}{n} \sum_{i \in [n]} \frac{1}{N^{1/p}} \left\| (I - \Pi)y^{(i)} \right\|_p$$

(34)
B Synthetic Data Experiments

If we extend the collection of continuous functions in $C_X$ (Section 3.3) to the measurable functions, and take as distance $d$ the one induced from the $L_2$ norm on random variables, then the $Z \in C_X$ that minimizes $\rho(Y|X)$ is almost everywhere equivalent to conditional expectation $\mathbb{E}[Y|X]$. Consequently, conditional expectation $\mathbb{E}[Y|X]$ can be used for testing $\rho(Y|X)$ values on synthetic data.

1D. To demonstrate the ability of recoverability to capture the existence of a continuous map from one random variable to another, we use a simple 1D experiment. Let $X$ be a normally distributed random variable, and let $Z$ and $W$ be defined as follows:

$$Z = f_1(X) = \text{sign}(X) \cdot X^2$$

$$W = f_2(X) = X^2.$$  \hspace{1cm} (35)

Since $f_1$ is invertible and $f_2$ is not, we can fully recover $X$ from $Z$ but not from $W$. Of course, we can fully recover $Z$ and $W$ from $X$, since we explicitly defined continuous maps $f_1$ and $f_2$.

For this test we generated 1000 samples of $X$ and estimated $\rho$ using Theorem 2. The results are shown in Table 3.

Theoretical recoverability loss for Table 3.

$$\mathbb{E}[Z|X] = Z \Rightarrow \rho(Z|X) = \sqrt{\mathbb{E}[(Z - Z)^2]} = 0$$  \hspace{1cm} (37)

$$\mathbb{E}[X|Z] = X \Rightarrow \rho(X|Z) = \sqrt{\mathbb{E}[(X - X)^2]} = 0$$  \hspace{1cm} (38)

$$\mathbb{E}[W|X] = W \Rightarrow \rho(W|X) = \sqrt{\mathbb{E}[(W - W)^2]} = 0$$  \hspace{1cm} (39)

$$\mathbb{E}[X|W = w] =$$

$$= \mathbb{E}[\mathbb{1}_{X \geq 0}X|W = w] + \mathbb{E}[\mathbb{1}_{X < 0}X|W = w] =$$

$$= \mathbb{E}[\mathbb{1}_{\sqrt{w} \geq 0}\sqrt{w}] + \mathbb{E}[\mathbb{1}_{\sqrt{w} < 0}(-\sqrt{w})] = 0$$  \hspace{1cm} (40)

$$\rho(X|W) = \sqrt{\mathbb{E}[(X - 0)^2]} = 1$$  \hspace{1cm} (41)

100D. Now, let $X$ and $N$ be 100-dimensional random vectors, with independent normally distributed entries. $Y$ be defined as

$$Y = \sum_{i \in [100]} (X_i + \alpha \cdot N_i),$$  \hspace{1cm} (42)

where $\alpha$ is some parameter. When $\alpha$ tends to zero, $Y$ can be fully recovered from $X$, and when $|\alpha|$ is large, the noise $N$ dominates the value of $X$; consequently, $Y$ cannot be recovered from $X$. This behavior is visualized in Fig. 5, where $\rho(Y|X)$, estimated on 1000 samples, is compared to its theoretical value.

Theoretical recoverability loss for Fig. 5.

$$\mathbb{E}[Y|X = x] = \sum_{i \in [100]} (x_i + \alpha \cdot N_i) = \sum_{i \in [100]} x_i$$  \hspace{1cm} (43)

$$\mathbb{E}[Y|X] = \sum_{i \in [100]} X_i$$  \hspace{1cm} (44)

$$\rho(Y|X) = \sqrt{\mathbb{E}[(Y - \sum_{i \in [100]} X_i)^2]} = |\alpha|\sqrt{100}$$  \hspace{1cm} (45)

C Dataset Statistics

The datasets used in our experiments are given in Table 4.
Table 3: The estimated distance from $X$ to $C_W$ is larger than the distance from $X$ to $C_Z$, since we cannot fully recover $X$ from $W$.

|       | $\hat{\rho}$ | $\rho$ |
|-------|--------------|--------|
| $\rho(X|Z)$ | 0.119 ± 0.004 | 0      |
| $\rho(X|W)$ | 0.974 ± 0.026 | 1      |
| $\rho(Z|X)$ | 0.099 ± 0.013 | 0      |
| $\rho(W|X)$ | 0.110 ± 0.019 | 0      |

Figure 5: Comparison between estimated $\rho(Y|X)$ and its theoretical values for different $\alpha$.

| Name            | Type        | Nodes | Edges    |Feat. dim.| Classes | Multilabel |
|-----------------|-------------|-------|----------|----------|---------|------------|
| Cora [69]       | Transductive | 2,708 | 5,429    | 1,433    | 7       | –          |
| Citeseer [69]   | Transductive | 3,327 | 4,732    | 3,703    | 6       | –          |
| PubMed [69]     | Transductive | 19,717| 44,324   | 500      | 3       | –          |
| DBLP [17]       | Transductive | 17,716| 105,734  | 1,639    | 4       | –          |
| Amazon-Photos [61] | Transductive | 7,650 | 119,081  | 745      | 8       | –          |
| Reddit [22]     | Inductive   | 232,965| 57,307,946| 602      | 41      | –          |
| Reddit2 [21]    | Inductive   | 232,965| 11,606,919| 602      | 41      | –          |
| ogbn-arxiv [27] | Inductive   | 169,343| 1,166,243 | 128      | 40      | –          |
| PPI [78]        | Inductive   | 56,944 | 793,632  | 50       | 121     | ✓          |
| ogbn-products [27] | Inductive   | 2,449,029| 61,859,140| 100      | 47      | –          |

Table 4: Dataset statistics.
Figure 6: Comparison of test accuracy in the downstream tasks of the self-supervised setup and random initial setup, where in the random initial setup, the self-supervised training was skipped. Each column refers to a different dataset. Each row corresponds to a different GNN layer type.

D Additional Experimental Results

In Fig. 6 we demonstrate the results for the GraphConv and SAGEConv layers, that are related to the ablation study in Section 4.3.