IMPROVING OUT-OF-DISTRIBUTION GENERALIZATION WITH INDIRECTION REPRESENTATIONS

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ABSTRACT

We propose a generic module named Indirection Layer (InLay), which leverages indirection and data internal relationships to effectively construct symbolic indirect representations to improve out-of-distribution generalization capabilities of various neural architectures. InLay receives data input in the form of a sequence of objects, treats it as a complete weighted graph whose vertices are the objects and edge weights are scalars representing relationships between vertices. The input is first mapped via indirection to a symbolic graph with data-independent and trainable vertices. This symbolic graph is then propagated, resulting in new vertex features whose indirection will be used for prediction steps afterward. Theoretically, we show that the distances between indirection representations are bounded by the distances between corresponding graphs, implying that unseen samples with very different surface statistics can still be close in the representation space to the seen samples if they share similar internal relationships. We demonstrate that InLay is consistently effective in improving out-of-distribution generalization throughout a comprehensive suite of experiments, including IQ problems, distorted image classification, and few-shot domain adaptation NLP classification. We also conduct ablation studies to verify different design choices of InLay.

1 INTRODUCTION

There have been several evidences showing that deep learning models may fail drastically in out-of-distribution (OOD) testing circumstances (Geirhos et al., 2018; Keysers et al., 2020). One reason widely agreed upon is that neural networks tend to learn surface statistics of data (Lake et al., 2017) and thus can not generalize to new samples with different statistics. On the other hand, humans excel at generalizing, and it has been long believed that the ability to think in a symbolic way is the key for humans to quickly adapt to new situations (Mitchell, 2021). A powerful concept that can bridge concrete data and symbols is indirection, which binds two objects together and uses one to refer to the other. In computer science, indirection is widely used via pointer: data is bound to its memory address, and programs use the memory address to refer to that data.

The capacity to draw analogies is yet another trait that facilitates human generalization. Several cognitive science theories have been proposed to explain analogy, and the Structure-Mapping Theory (SMT) (Gentner, 1983) is one of the most successful among them. SMT argues that not object attributes but the relationships between them are transferred in an analogy. For example, the hydrogen atom is analogous to the solar system not because they share the same sizes or temperatures but because they both have entities revolving around a center due to the attractive force. This suggests that internal relationships of a situation contain essential information for generalization. In this paper, we propose a method that simultaneously leverages indirection and data internal relationships to construct *indirection representations*, which can be interpreted as symbolic representations that respect the similarities *between* internal relationships. For instance, two IQ problems with similar hidden rules (i.e., similar internal relationships) should have similar indirection representations, though they contain completely different shapes or images.

To this end, we implement our method in the form of a generic module named Indirection Layer (InLay), which can construct indirection representations from either encoded or raw low-sensory data and can be equipped with various models to improve their OOD generalization capabilities. InLay receives a sequence of objects as input and produces a sequence with the same length including associated indirection representations. The input sequence is viewed as a complete weighted graph

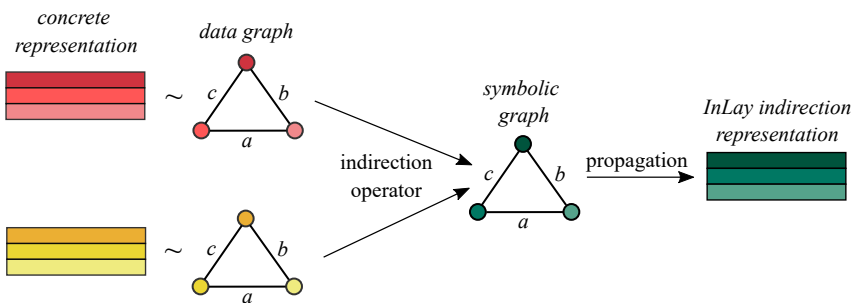


Figure 1: *Indirection Layer*. Concrete data representation is viewed as a complete graph with weighted edges. The indirection operator maps this graph to a symbolic graph with the same weight edges, however the vertices are fixed and trainable. This symbolic graph is propagated and the updated node features are indirection representations. Different concrete inputs may share the same indirection representations if their corresponding graphs have the same adjacency matrices. This illustrates the core idea of InLay: constructing indirection representations by transferring internal relationships through indirection.

where each edge weight represents the relationship between two corresponding objects, and thus the adjacency matrix of this graph captures the internal relationships of the input. The core operation of InLay consists of two steps: indirection and graph propagation (see Fig. 1 for illustration). The input is first processed through indirection to transfer all edge weights to another symbolic graph whose vertices are data-independent and trainable. This symbolic graph is then propagated, resulting in updated vertex features as the indirection representations of the input. These indirection representations are used as new representations for prediction steps afterward.

We show both theoretically and empirically that InLay can help to improve OOD generalization. Theoretically, we show that InLay indirection preserves internal structures of graphs and the global structure of graph space. In addition, the distances between indirection representations are bounded by the distances between corresponding graphs. Thanks to these theoretical properties, the indirection representation of a new data instance can be located near a seen one if they share similar internal relationships, thus the two instances have a higher chance of being interpreted similarly. Empirically, we show that InLay consistently helps different models to improve their OOD generalization capabilities in a comprehensive suite of experiments involving numerous datasets and OOD scenarios, including IQ problems with unseen objects and unseen rules, distorted image classification, and few-shot domain adaptation NLP classification. We also conduct ablation experiments to study the necessity of different design choices in InLay and provide practical analysis on the success of InLay.

2 Method

This section introduces our main contribution, namely the Indirection Layer (InLay). InLay takes a sequence of objects as input and transforms the sequence into a new indirect graph-structured representation. Concretely, let $X = (x_1, x_2, \ldots, x_k)^\top \in \mathbb{R}^{k \times n}$ as the input sequence for InLay, where k is the number of objects and each $x_i \in \mathbb{R}^n$ represents for an object. For example, an object may be either an image in IQ problems, or a patch of image in image classification task, or a paragraph in few-shot NLP classification task (see Section 4 for more details). To better exploit data internal relationships, we treat each input sequence as an undirected complete weighted graph whose vertices are the objects and edges represent relationships as a scalar in $[-1, 1]$. Specifically, for each sequence X, we denote G_X as its corresponding graph. We define $\mathcal{G}_k$ to be the space of all undirected weighted complete graphs G with k vertices, and all edge weights belong to $[-1, 1]$. From now on, we will only write G instead of G_X when it is not necessary to specify X, and we denote A_G as the adjacency matrix of G. This adjacency matrix captures the internal relationships of the corresponding data sequence.

We aim to learn suitable representations for the graph such that the internal relationships of the input sequence can be transferable to novel settings. To this end, we contribute the Indirection Layer (InLay), which leverages indirection and data internal relationships to construct indirection representations. InLay is a generic and flexible module that can be equipped with different models to construct indirection representations from either encoded data or raw low-sensory data (e.g, for the case of Vision Transformer; see Section 4.2) in two steps: indirection and graph propagation.

Indirection

For each X, the adjacency matrix $A_{G_X} = \left(a_{ij}^X\right)_{i,j=\overline{1,k}} \in \mathbb{R}^{k\times k}$ of G_X represents the internal relationships between objects in X. Each component a_{ij}^X of A_{G_X} is computed as $a_{ij}^X = \tanh\left(\frac{Q^\top x_i \cdot K^\top x_j}{\sqrt{4n}}\right)$, where $\cdot$ is the inner product and $Q, K \in \mathbb{R}^{n\times 4n}$ are trainable weights that project x_i and x_j onto a higher dimensional space so that a linear kernel may represent the relationship between x_i and x_j. The choice of tanh as a non-linear transformation is important: it maps the dot products to $[-1, 1]$, allowing InLay to possess nice theoretical properties regarding boundedness of distances (see Section 3); and, tanh allows negative similarities between objects, which may help to represent opposite relations, e.g., translations to the left and to the right. See Section 4.1.1 for more experimental details.

In indirection, each object is bound to a symbol. We denote by $V^{\text{ind}} = \left(v_1^{\text{ind}}, v_2^{\text{ind}}, \ldots, v_k^{\text{ind}}\right)^\top \in \mathbb{R}^{k\times n}$ to be the set of symbols where each $v_i^{\text{ind}} \in \mathbb{R}^n$ is data-independent and trainable. Let $\mathcal{G}_k^{\text{ind}}$ be the subset of $\mathcal{G}_k$ that consists of all graphs whose set of vertices is V^{ind}. The space $\mathcal{G}_k^{\text{ind}}$ can be interpreted as the space of symbolic graphs with fixed vertices. We define the indirection operator $\mathcal{I}$ as follows.

Definition 2.1. Given a map $G \in \mathcal{G}_k$ with vertices $(x_1, x_2, \ldots, x_k)$. The *indirection operator* $\mathcal{I}$ is a mapping from $\mathcal{G}_k$ to $\mathcal{G}_k^{\text{ind}}$ that maps G to $\mathcal{I}(G) \in \mathcal{G}_k^{\text{ind}}$ so that x_i is mapped to v_i^{ind} and $A_G = A_{\mathcal{I}(G)}$.

The indirection operator $\mathcal{I}$ maps each object x_i to its associated symbol v_i^{ind} while assuming the pairwise relationship between v_i^{ind} and v_j^{ind} is the same as one between x_i and x_j (see Fig. 1). That is, $\mathcal{I}$ ignores the concrete features of objects but still maintains the relationships between them.

Graph propagation

After indirection, each graph G is mapped to a symbolic graph $\mathcal{I}(G)$. Things can be interpreted as follows: at first, $\mathcal{I}(G)$ does not contain edge weights; then the indirection operator $\mathcal{I}$ brings edge weights from the data to $\mathcal{I}(G)$. Once receiving this information from data, $\mathcal{I}(G)$ is propagated and the updated vertex features are indirection representations of the input sequence. Formally, for an input sequence X, if we denote r_X to be the indirection representations of X, then $r_X = A_{G_X} V^{\text{ind}}$. This symbolic r_X is used as a new representation for X for prediction steps afterward.

To summarize, for each input sequence X, InLay constructs associated indirection representation r_X:

$$r_X = \tanh\left(\frac{XQ(XK)^\top}{\sqrt{4n}}\right) V^{\text{ind}}. \tag{1}$$

This equation is closely related to self-attention, except for three points: 1. data are projected onto a higher dimensional space by matrix multiplying with Q and K; 2. the softmax operator is replaced by tanh; and most importantly, 3. the value V^{ind} is **not** computed based on the data X. While the first two differences empirically enhance InLay's performances (see Section 4.4), the third one stands for the core idea of indirection in InLay. An ablation study on V^{ind} will also be given in Section 4.4.

Initialization of V^{ind} may greatly affect the overall performance. To reduce this effect, we replace V^{ind} in Eq. (1) by $\psi(V^{\text{ind}})$, where $\psi : \mathbb{R}^n \to \mathbb{R}^n$ is a trainable 2-layer neural network applied to rows of V^{ind}. We also use multi-heads to compute the adjacency matrix so that local information of feature vectors is better utilized. The number of heads is tuned for each specific task.

3 Theoretical Analysis

Graph spectrum and Laplacian are important graph characteristics that, in the case of complete graphs, can be computed entirely by graph adjacency matrices. From Definition 2.1, it obviously follows that the indirection operator $\mathcal{I}$ preserves graph spectrum and Laplacian, which means $\mathcal{I}$ preserves graph internal structure. To some extent, this agrees with the Structure-Mapping Theory (Gentner, 1983), which states that not the attributes but the internal relationships are transferred in an analogy. In other words, learning internal relationships may already be enough to capture the essence of a situation. Further details for the Structure-Mapping Theory will be given in Section 5.

Next, we investigate how distances between graphs may constrain distances between indirection representations. Before defining graph distance, we define isomorphism between graphs in $\mathcal{G}_k$.

Definition 3.1. Given two graphs $G = (V, E) \in \mathcal{G}_k$ and $G' = (V', E') \in \mathcal{G}_k$ with associated adjacency matrices $A_G = (a_{ij})_{i,j=\overline{1,k}}$ and $A_{G'} = (a'_{ij})_{i,j=\overline{1,k}}$. We say G and G' are *isomorphic*, denote by $G \cong G'$, if there exists a bijection $\phi : V \to V'$ so that $a_{ij} = a'_{\phi(i)\phi(j)}$ for every $i, j \in V$.

Two isomorphic graphs can be interpreted to be identical up to isomorphism, and thus a graph distance defined on $\mathcal{G}_k$ should respect this property, i.e., the distance between two isomorphic graphs is 0. One such distance is the rectangle distance $\hat{\delta}_\square$, which is a useful tool for studying the convergence of sequence of graphs. Specifically, it has been shown that graph convergence with respect to homomorphism density is equivalent to graph convergence with respect to the distance $\hat{\delta}_\square$. Readers are referred to (Borgs et al., 2008) for more details. A formal definition for $\hat{\delta}_\square$ is given in Appendix A.

From the definition of $\hat{\delta}_\square$, it is clear that $\hat{\delta}_\square(G, G') = 0$ if and only if G is isomorphic with G'. Moreover, if $G_1 \cong G_2$ then $\hat{\delta}_\square(G_1, G') = \hat{\delta}_\square(G_2, G')$ for any $G' \in \mathcal{G}_k$. Since $G \cong \mathcal{I}(G)$, this leads to the fact that the indirection operator $\mathcal{I}$ preserves $\hat{\delta}_\square$ distance, i.e., $\hat{\delta}_\square(G, G') = \hat{\delta}_\square(\mathcal{I}(G), \mathcal{I}(G'))$ for every $G, G' \in \mathcal{G}_k$. This means $\mathcal{I}$ preserves any topology on $\mathcal{G}_k$ induced from $\hat{\delta}_\square$, which shows that $\mathcal{I}$ preserves the global structure of the graph space $\mathcal{G}_k$.

We have shown that the indirection operator $\mathcal{I}$ admits some invariant properties with respect to the graph spectrum, Laplacian and the rectangle graph distance $\hat{\delta}_\square$. That is to say, $\mathcal{I}$ respects the graph internal structure, and it does not lose topological properties of the concrete graph space when mapping to the symbolic graph space. The following results will instead focus on the local properties in graph spaces, that is, how the distance between two graphs may affect the distance between the indirection representations produced by InLay as in Eq. (1). For each $G \in \mathcal{G}_k$, we denote $r_G = A_G V^{\text{ind}}$ to be its associated indirection representation.

Theorem 3.2. *For any two graphs $G \in \mathcal{G}_k$ and $G' \in \mathcal{G}_k$, the following inequality holds:*

$$\|r_G - r_{G'}\|_\infty \leq \left(2 + k^2 \hat{\delta}_\square(G, G')\right) \|V^{ind}\|_\infty, \tag{2}$$

where $\|.\|_\infty$ is the max norm on $\mathbb{R}^n$. If G and G' are isomorphic, then $\|r_G - r_{G'}\|_\infty \leq 2\|V^{ind}\|_\infty$.

Proof. See Appendix B. □

Note that even when $\hat{\delta}_\square(G, G') = 0$, r_G may still be different from $r_{G'}$. This is because by design, InLay also takes into account the ordinal information of input sequence, which may be important in some specific use cases, e.g., when the input is sequence of image patches. Theorem 3.2 shows that if G and G' are close, their indirection representations will not be far away from each other as well. This is an important property since the original vertex representations of G and G' may be arbitrarily far though G and G' are isomorphic, e.g., two IQ problems with the same hidden rules but different images may be represented very differently. Theorem 3.2 also shows the necessity of training V^{ind} to obtain appropriate $\|V^{\text{ind}}\|_\infty$: if $\|V^{\text{ind}}\|_\infty$ is too large, the bound in Ineq. (2) is loose; conversely, if $\|V^{\text{ind}}\|_\infty$ is too small, the bound may be too strict so that indirection representations are not well separated enough. An empirical ablation study on V^{ind} will be given in Section 4.4.

Theorem 3.2 focuses on the distance between two single indirection representations. Now we move our attention to the distance between sets of indirection representations associated with isomorphic classes of graphs. For each $G \in \mathcal{G}_k$, denote $R_G = \{r_{\tilde{G}} : \tilde{G} \in \mathcal{G}_k, \tilde{G} \cong G\}$. According to Theorem 3.2, diam $R_G \leq 2\|V^{\text{ind}}\|_\infty$ for every $G \in \mathcal{G}_k$, where diam stands for the diameter of a set. We now focus on the distance between R_G and $R_{G'}$, and we use the popular Hausdorff metric to measure this distance. The distance between R_G and $R_{G'}$ is meaningful in the sense that for any $r' \in R_{G'}$, we can find $r \in R_G$ so that $\|r - r'\|_\infty \leq d_H(R_G, R_{G'})$. This means if r' is the indirection representation of a novel situation, it can be located close to some observed r. The following last theorem shows that the Hausdorff distance d_H with respect to the $\|.\|_\infty$ norm between R_G and $R_{G'}$ also depends on the distance between G and G'.

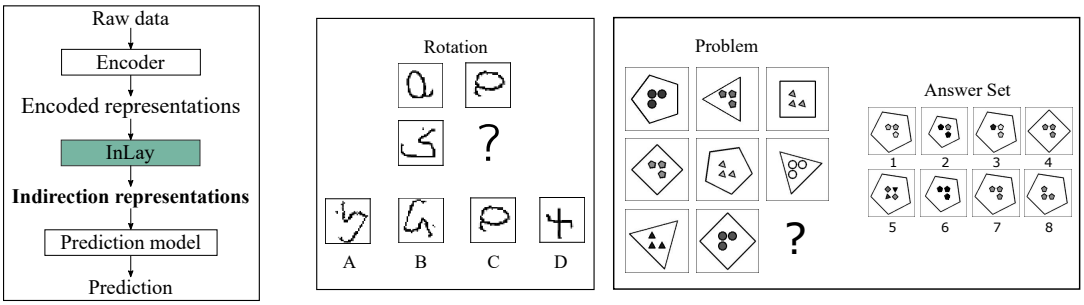
Theorem 3.3. *Given two graphs $G \in \mathcal{G}_k$ and $G' \in \mathcal{G}_k$. The following inequality holds:*

$$d_H(R_G, R_{G'}) \leq k^2 \|V^{ind}\|_\infty \hat{\delta}(G, G'). \tag{3}$$

Moreover, if G and G' are not isomorphic and rank $V^{ind} = k$, then $R_G \cap R_{G'} = \varnothing$.

Proof. See Appendix B. □

Theorem 3.3 shows that InLay partitions the indirection representation space into disjoint subsets, each of which corresponds to a class of isomorphic graphs, and the distances between these subsets



(a) (b)

Figure 2: **(a)** Overall architecture of prediction model when equipped with InLay**.** **(b)** *Left:* A problem in FINE dataset with images from the Omniglot dataset and hidden rule is 90-degree rotation. *Right:* A Raven's Progressive Matrix problem from RAVEN dataset. Images adapted from original papers.

are still bounded by the original graph distances. Intuitively, these results explain why InLay may help models deal with new situations: if the new situation is related to seen data, its indirection representation is also close to one of that seen data, thus the prediction model has a better chance of drawing an analogy between them. An illustration for theoretical results is given in Appendix B.

4 Experiments

In this section, we conduct several experiments with different scenarios of OOD generalization to show that InLay can adapt to various models and improve their performances on various datasets. The OOD testing scenarios are IQ problems with unseen images and unseen rules, distorted image classification, and domain adaptation on few-shot NLP classification, all of which require the ability to understand the problem in a systematic and symbolic way in order to generalize on new OOD circumstances. Throughout these experiments, we show that InLay consistently helps models to perform better. We also provide an ablation study on the necessities of different design choices in InLay, as well as a practical analysis of the success of InLay.

InLay constructs indirection representations from either encoded or raw data. If the prediction model is equipped with an encoder, InLay will lie between the encoder and prediction to transform encoded representations to indirection representations (see Fig. 2a for an illustration). When there is no encoder, e.g., when the prediction model is Vision Transformer, InLay directly constructs indirection representations from raw data. To be fair when comparing, models with or without InLay are all trained with the same training settings, including batch size, learning rate, number of training iterations, optimizer, etc., and we only report test results after the last iteration. Average results are reported in the main text; full results with standard deviation are given in Appendix C. More training details are also given in Appendix E.

In practice, we optionally use context normalization (Webb et al., 2020a) to further improve InLay. Context normalization is a normalization technique that normalizes along the contextual dimension and has been shown to be effective in out-of-distribution scenarios. If context normalization is applied in InLay, there will be two such layers: one to normalize the original representation X, and one to normalize the symbolic representation r_X.

4.1 Out-of-distribution IQ Problems

IQ problems are powerful testbeds for OOD generalization capability of deep learning models. Despite their simple appearances, IQ problems are challenging in the sense that they require models to understand the hidden rules instead of just surface features to solve new problems with unseen objects or even unseen (but related) rules. There has been evidence showing that current deep learning models may fail when facing problems with unseen objects (Webb et al., 2020b). In this experiment, we show that models coupled with InLay achieve better performances on two IQ datasets: FINE (Pham et al., 2022) and RAVEN (Zhang et al., 2019). Examples are given in Fig. 2b.

4.1.1 FINE Dataset

FINE dataset consists of IQ problems with geometric transformations as hidden rules. To succeed in this dataset, models should treat objects as symbols and learn the relationship between these symbols. Here we consider one of the most challenging OOD scenarios: test problems include unseen objects

Train set Test set	CIFAR100 Omniglot				MNIST CIFAR100			
	Trans.	Rot.	Shear	Scale	Trans.	Rot.	Shear	Scale
NTM	25.5/**56.9**	27.1/**31.4**	29.8/**58.5**	30.3/**61.0**	35.2/**69.2**	30.0/**34.5**	29.6/**56.0**	31.9/**48.7**
PrediNet	26.7/**28.5**	25.5/**28.3**	25.6/**29.0**	26.4/**29.9**	27.5/**31.6**	26.8/**27.8**	26.4/**28.4**	33.6/**35.9**
RelationNet	25.4/**39.3**	25.0/**34.0**	25.1/**39.8**	24.7/**50.2**	25.6/**45.5**	25.6/**35.2**	25.0/**43.4**	26.8/**44.8**
Transformer	26.9/**63.3**	27.2/**40.4**	28.3/**65.3**	30.6/**62.0**	37.8/**63.9**	32.0/**36.1**	30.2/**53.5**	29.2/**48.1**

Table 1: Average test accuracy (%) without/with InLay on FINE dataset.

Train configuration Test configuration	Up-Down Left-Right	3x3Grid 2x2Grid	Out-InGrid Out-InCenter	Average
LSTM	28.8/**43.9**	19.5/**25.1**	42.1/**48.6**	30.1/**39.2**
Transformer	15.2/**56.7**	13.6/**26.0**	16.6/**44.7**	15.1/**42.5**
RelationNet	12.7/**58.5**	12.4/**28.9**	12.3/**51.7**	12.5/**46.4**
PrediNet	13.7/**16.5**	13.6/**14.3**	14.2/**15.9**	13.8/**15.6**

Table 2: Average test accuracy (%) without/with InLay on RAVEN dataset.

and unseen rules. To be specific, images in train and test problems come from different datasets (train on CIFAR100 (Krizhevsky, 2009) - test on Omniglot (Lake et al., 2015) or train on MNIST (LeCun et al., 2010) - test on CIFAR100), so the models need to understand the hidden rules instead of image features to solve test problems. Rules in test problems are also unseen during training; for instance, we train on IQ problems with rotation angle less than 180° and test on ones with rotation angles more than 180°; similarly, for translation, we train on problems with translation to the left and test on ones with translation to the right. More details of other transformations will be given in Appendix. Models to be considered include the Neural Turing Machine (Graves et al., 2014), PrediNet (Shanahan et al., 2020), Relation Network (Sung et al., 2018), and Transformer (Vaswani et al., 2017), all of which have been shown to be effective on different relational reasoning tasks. All models, with or without InLay, are equipped with context normalization. Results are reported in Table 1.

Overall, models perform better when equipped with InLay, even in very extreme cases when models are trained on grayscale MNIST images and tested on RGB CIFAR100 images. This shows a clear advantage of InLay: indirection maps concrete features to symbolic space spanned by V^{ind}, thus helping models to be less dependent on concrete data. It can also be observed that PrediNet equipped with InLay improves less than other models. This is because PrediNet also constructs new symbolic data representations, and thus contains the inductive bias of symbolic representations itself. Again, this emphasizes the necessity of including symbolic inductive bias to improve OOD generalization.

4.1.2 RAVEN DATASET

RAVEN dataset (Zhang et al., 2019) is inspired by Raven's Progressive Matrices, which are challenging IQ tests for humans. RAVEN IQ problems are complex in the sense that a single problem may consist of different shapes, each of which follows a different rule. Inspired by the original paper, we conduct experiments to test models' capabilities to generalize on problems of unseen configurations. Specifically, we train and test on problems of different but related configurations. For example, Up-Down problems are related to Left-Right ones in the sense that Left-Right configuration can be viewed as a 90-degree "rotation" of Up-Down. In this experiment, the three train-test configuration pairs are UpDown-LeftRight, 3x3Grid-2x2Grid and OutInGrid-OutInCenter. We also apply context normalization in all models. We further apply Dynamic Residual Tree as proposed in the original paper to capture the inherent structure of Raven's Progressive Matrices. Results are reported in Table 2. A similar pattern can be observed: models equipped with InLay tend to perform better. In average, InLay helps improve LSTM by 9.1%, Transformer by 27.4%, RelationNet by 33.9%, and PrediNet by 1.8%. This can be well explained by Theorem 3.2 and Theorem 3.3 in the theoretical analysis: although the test configuration is unseen, it is still related to the train configuration and thus InLay representations for test problems may still be close to ones of train problems. This helps models to have a better chance to draw analogies between observed and unobserved configurations.

4.2 OUT-OF-DISTRIBUTION CLASSIFICATION

Humans can consistently recognize objects in different positions, angles, or colors. Current deep learning models may not. Geirhos et al. (2018) show that when test images are injected with different kinds of distortions other than ones in training, deep neural networks may fail drastically on image

Dataset	Image transformation		Color transformation				Average
	Rot90	VFlip	Jitter	Invert	Blur	Grayscale	
SVHN	**16.4**/15.8	34.1/**35.3**	85.7/**90.2**	85.7/**90.1**	86.4/**89.8**	86.9/**91.8**	65.9/**68.8**
CIFAR10	25.7/**27.9**	32.1/**35.0**	23.2/**24.9**	39.4/**48.3**	**60.2**/59.5	48.3/**62.7**	38.2/**43.1**
CIFAR100	13.4/**15.0**	13.5/**16.8**	6.6/**9.7**	19.4/**23.4**	33.4/**33.5**	16.4/**23.9**	17.1/**20.4**

Table 3: Average test accuracy (%) without/with InLay on OOD classification task with ViT.

	ProtoNet	SNAIL	GNN	MTB
5-way-1-shot	64.7/**65.4**	38.6/**60.6**	36.7/**63.1**	66.1/**68.9**
10-way-1-shot	**49.1**/41.7	17.3/**34.9**	27.1/**43.3**	52.9/**54.1**
Average	**56.9**/53.6	28.0/**47.8**	31.9/**53.2**	59.5/**61.5**

Table 4: Average validation accuracy (%) without/with InLay on FewRel 2.0.

classification tasks. We take inspiration from that result and conduct similar experiments to test whether InLay can help models improve their performances on OOD image classification tasks. We use a vanilla 6-layer Vision Transformer (ViT) (Dosovitskiy et al., 2020) as the base model and test it, with or without InLay, on different datasets, namely the SVHN (Netzer et al., 2011) and CIFAR10&100 (Krizhevsky, 2009). The models are trained on original images with no data augmentation and tested on images with various distortions, including image transformations (90-degree rotation, vertical flip) and color transformations (color jitter, color invert, blur, and grayscale). If InLay is equipped, we divide each 32×32 image into overlapping patches of size 8×8 and stride 4. These patches are vertices of the graph that represents the current image. The patch indirection representations are reassembled to form a new image of the same size as the original one. This new image is then fed into ViT. Context normalization is not used in this task.

Results are shown in Table 3. As expected, ViT performs poorly when the images are distorted. In average, InLay helps to improve its performance by 2.9% on SVHN, 4.9% on CIFAR10, and 3.3% on CIFAR100. Note that while the equation of InLay is closely related to self-attention, it should not be interpreted that adding InLay to ViT is equivalent to adding a Transformer layer. Empirically, performances of 7-layer ViT only slightly differ from 6-layer ViT (see Appendix D), while it is clear that adding InLay may boost performances significantly.

4.3 Few-shot NLP Domain Adaptation

Humans can handle NLP classification tasks given a small number of examples. While humans can quickly adapt to such new scenarios, deep language models may not. Gao et al. (2019) proposed the FewRel 2.0 dataset that consists of few-shot NLP classification tasks, where the domains of train and test tasks vastly differ. Specifically, the training texts are taken from the Wikipedia corpus, while texts for testing originate from the PubMed and UMLS databases that contain large amounts of biomedical literature and sciences. This creates a big obstacle for few-shot language models to adapt to: their performances drop drastically as reported in the original paper.

Inspired by this result, we conduct an experiment on FewRel 2.0 dataset to show that InLay still fits well for language models. Different few-shot models, including Prototypical Network (Snell et al., 2017), SNAIL (Mishra et al., 2017), Graph Neural Network (Garcia and Bruna, 2017), and MTB (Soares et al., 2019), are trained with BERT encoder (Devlin et al., 2018) on 5-way-1-shot and 10-way-1-shot tasks. All models are equipped with context normalization. Since the test set is not provided for the public, we only report the test results on validation set, which shares the same domain as the test set. Results are shown in Table 4. Except ProtoNet, InLay helps other models improve: 19.8% for SNAIL, 21.3% for GNN, and 2.0% for MTB in average. The case of ProtoNet can be explained as follows: ProtoNet does not depend on concrete features but only the distances between them, which is similar to the spirit of our InLay. Because ProtoNet already has this inductive bias, InLay can not help to improve it.

4.4 Ablation and Analysis

4.4.1 Ablation on InLay Design Choices

We conduct ablation experiments to study the necessities of different design choices of InLay. All experiments are conducted on OOD classification task (see Section 4.2) with ViT and grayscale testing images. In each experiment, we modify one design choice and keep others fixed. We consider

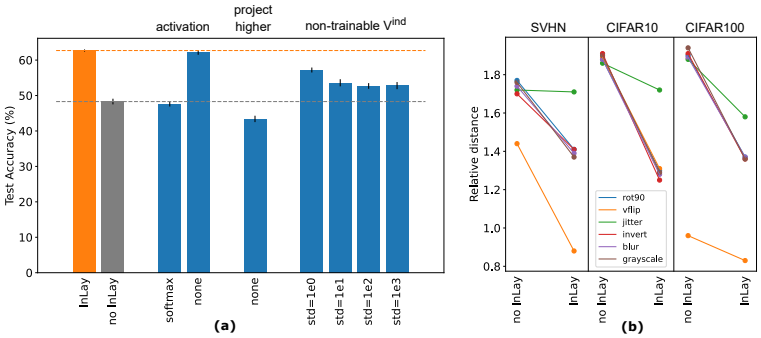


Figure 3: **(a)** *Ablation study.* Test accuracies of ViT equipped with InLay on grayscale images when a design choice of InLay is replaced or removed. **(b)** Relative distances between original and distorted representations with and without InLay in different testing cases.

three main design choices: activation function to compute adjacency matrices, projection on higher space to compute dot products, and trainability of V^{ind}. Results are reported in Fig. 3a.

In the ablation for activation function, replacing tanh with softmax significantly decreases the performance, while the result when no activation is applied is only slightly lower. This is because softmax does not allow negative values; moreover, it imposes the constraint of summing-to-one on edges of graph, which is unnecessary in the theoretical analysis. On the other side, projecting data onto higher dimensional spaces also plays a vital role in InLay as it helps linearize the relations between objects so that dot products may manage to represent those relations, and not doing so may lead to a drastic drop in performance. Finally, maintaining a trainable set of symbols V^{ind} is beneficial for InLay, and the performances with randomly sampled V^{ind} from Gaussian tend to decrease when the standard deviations of the Gaussians increase. This can be explained by Theorem 3.2: increase of standard deviations leads to bigger $\|V^{\text{ind}}\|_\infty$, which loosens the bound in Ineq. (2).

4.4.2 Further Practical Analysis

Besides theoretical analysis in Section 3, we further provide practical evidence showing why InLay may help models to generalize better. We again use the OOD classification tasks as a testbed. In short, we would like to show that InLay reduces the distance between an image and its distorted version, thus models may recognize the similarity between the two images more easily. Using the absolute distance may not be a fair metric since scaling two vectors by the same factor may already reduce the distance between them. Instead, we compute the relative distances between vectors, i.e. the relative distance between u and v is $2 \times \frac{\|u-v\|_\infty}{\|u\|_\infty + \|v\|_\infty}$. Relative distances between images and their distorted versions are computed in two cases: with InLay and without InLay. Results are shown in Fig. 3b, and it is clear that the relative distances in InLay case are lower than those without InLay. This can be partly explained by Theorem 3.2: the original image corresponds with G, and the distorted image corresponds with G'. Since the distorted image is closely related to the original one, the distance between their corresponding graphs is small, and thus the distance between their indirection representations r_G and $r_{G'}$ also tends to be small according to Ineq. (2).

5 Related Work

Systematic generalization has attracted attention recently in the deep neural networks community. One approach is to train a mixture of experts as functional modules, and these experts either compete (Parascandolo et al., 2018) or are composed by attention mechanism (Rahaman et al., 2021) to solve a task. Fedus et al. (2021) proposed the Switch Transformer to simplify routing algorithms in mixture-of-experts models to reduce communication and computational costs. Another approach is to design architectures that mimic human's ability to think and reason sequentially. One well-known early model following this approach is the Module Network (Andreas et al., 2016) which attacks the image-QA tasks by parsing the query into sequential sub-queries, each of which is solved by a module in the form of neural networks. The MAC recurrent network (Hudson and Manning, 2018) and the Neural State Machine (Hudson and Manning, 2019) follow a similar idea, however, in MAC the query is explicitly and expressively decomposed by a sequence of RNN-type MAC cells, while Neural State Machine relies on probabilistic graphs representing underlying semantics to reason sequentially. Recently, Wei et al. (2022) proposed the idea of chain of thought to improve

the ability of large language models to perform complex reasoning. Our InLay also follows the idea of injecting symbolic inductive bias, however, we focus on representations instead of functional modules. Models equipped with InLay can be interpreted as 2-step reasoning: the low-level sensory data is first represented symbolically by InLay, then processed by the following models.

Indirection is one of the most useful ideas that has been long applied in different areas of computer science. One of the most illustrative examples for indirection is the concept of pointer. Recently, there have been works leveraging indirection to improve generalization capabilities of deep learning models. ESBN (Webb et al., 2020b) uses an RNN controller to sequentially produce a symbolic key for each object and reasons on keys only. The keys in ESBN are computed based on the controller and similarities between objects, which is similar to our InLay; however, the keys are produced sequentially, which may increase the computational cost. Recently, Pham et al. (2022) proposed FINE, which is a fast-weight approach that utilizes indirection on functional spaces and has achieved promising performances on different OOD testing scenarios of IQ problems.

The idea of transferring relationships in InLay is inspired from the Structure Mapping Theory (SMT) (Gentner, 1983), which is a revolutionary theory of analogy in cognitive science. Analogy is a vital concept to explain human cognition, and it has been long argued that analogy-making underlies humans' ability to flexibly adapt to new situations (Gentner et al., 2001). Before SMT, it had been assumed that in a strong analogy, the base and the target should share several attributes in common (Tversky, 1977). SMT, in contrast, argues that not attributes but the relationships between objects are transferred in an analogy; in other words, the essence of a situation lies in internal relationships instead of concrete attributes. From this point of view, the theoretical results in Section 3 can be interpreted as a justification for SMT in the case of InLay: transferring relationships only does not lose significant information such as graph characteristics and graph topology.

Few-shot learning tasks are powerful testbeds for generalization capabilities of deep learning models. IQ problems, such as ones in FINE (Pham et al., 2022) or RAVEN (Zhang et al., 2019), can be viewed as few-shot learning tasks. There are several other IQ datasets that have been widely used as testbeds for visual reasoning and generalization, namely PGM (Barrett et al., 2018), ARC (Chollet, 2019), or Bongard-related datasets such as Bongard-LOGO (Nie et al., 2020) and Bongard-HOI (Jiang et al., 2022), all of which have been shown to be challenging in the visual domain. On the other side, the FewRel 2.0 dataset (Gao et al., 2019), which has been used in our experiments, is a popular dataset for NLP tasks. It is also worth noting that from few-shot learning perspective, our InLay can be categorized as fast-weight (Malsburg, 1994) embedding learning model, in which the attentional weight A_{G_X} is computed on-the-fly and the indirection representation r_X is computed accordingly.

The trainable set of symbols V^{ind} can be interpreted as a memory of positional encodings. From this point of view, the output r_X of InLay is a relative positional encoding regarding the input X. The idea of relative positional encoding (Shaw et al., 2018), as a replacement for the absolute positional encoding in Transformer, has been widely investigated and several variants have been proposed (Dai et al., 2019; Huang et al., 2018). It is worth noting that the relative positional encoding is added to the original input, while r_X in InLay plays the role of *the* input for the following model. InLay thus should not be considered as a variant of a Transformer layer or relative positional encoding; instead, its design highlights the idea of indirection and symbolic representations.

6 Conclusion

In this paper, we propose InLay as a separate module that can be plugged into different models to improve OOD generalization. InLay leverages the idea of indirection to redirect data representation based on a trainable set of symbols. Viewing each data point as a complete weighted graph, we prove theoretically that InLay preserves graph internal structure and graph topology, and the distances between refined representations are bounded by the distances between corresponding graphs. We show the effectiveness of InLay through a comprehensive suite of experiments, including different OOD testing scenarios on IQ problems, distorted image classification, and few-shot NLP domain adaptation classification tasks. We also conduct ablation experiments to study necessities of different design choices in InLay, as well as further practical analysis on the success of InLay.

InLay opens up several future directions. From the theoretical side, it is worth investigating how the manifold containing original data representations is transformed during InLay, and why this manifold transformation can help generalization. From the practical view, stacking multiple InLay's to form a hierarchical indirection network is a promising idea.

REFERENCES

Jacob Andreas, Marcus Rohrbach, Trevor Darrell, and Dan Klein. Neural module networks. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 39–48, 2016.

David Barrett, Felix Hill, Adam Santoro, Ari Morcos, and Timothy Lillicrap. Measuring abstract reasoning in neural networks. In *International conference on machine learning*, pages 511–520. PMLR, 2018.

Christian Borgs, Jennifer T Chayes, László Lovász, Vera T Sós, and Katalin Vesztergombi. Convergent sequences of dense graphs i: Subgraph frequencies, metric properties and testing. *Advances in Mathematics*, 219(6):1801–1851, 2008.

François Chollet. On the measure of intelligence. *arXiv preprint arXiv:1911.01547*, 2019.

Taco Cohen and Max Welling. Group equivariant convolutional networks. In *International conference on machine learning*, pages 2990–2999. PMLR, 2016.

Zihang Dai, Zhilin Yang, Yiming Yang, Jaime Carbonell, Quoc V Le, and Ruslan Salakhutdinov. Transformer-xl: Attentive language models beyond a fixed-length context. *arXiv preprint arXiv:1901.02860*, 2019.

Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. *arXiv preprint arXiv:1810.04805*, 2018.

Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, et al. An image is worth 16x16 words: Transformers for image recognition at scale. *arXiv preprint arXiv:2010.11929*, 2020.

William Fedus, Barret Zoph, and Noam Shazeer. Switch transformers: Scaling to trillion parameter models with simple and efficient sparsity, 2021.

Tianyu Gao, Xu Han, Hao Zhu, Zhiyuan Liu, Peng Li, Maosong Sun, and Jie Zhou. Fewrel 2.0: Towards more challenging few-shot relation classification. *arXiv preprint arXiv:1910.07124*, 2019.

Victor Garcia and Joan Bruna. Few-shot learning with graph neural networks. *arXiv preprint arXiv:1711.04043*, 2017.

Robert Geirhos, Carlos RM Temme, Jonas Rauber, Heiko H Schütt, Matthias Bethge, and Felix A Wichmann. Generalisation in humans and deep neural networks. *Advances in neural information processing systems*, 31, 2018.

Dedre Gentner. Structure-mapping: A theoretical framework for analogy. *Cognitive science*, 7(2): 155–170, 1983.

Dedre Gentner, Keith J Holyoak, and Boicho N Kokinov. *The analogical mind: Perspectives from cognitive science*. MIT press, 2001.

Alex Graves, Greg Wayne, and Ivo Danihelka. Neural turing machines. *ArXiv*, abs/1410.5401, 2014.

Cheng-Zhi Anna Huang, Ashish Vaswani, Jakob Uszkoreit, Noam Shazeer, Curtis Hawthorne, AM Dai, MD Hoffman, and D Eck. Music transformer: Generating music with long-term structure (2018). *arXiv preprint arXiv:1809.04281*, 2018.

Drew A. Hudson and Christopher D. Manning. Compositional attention networks for machine reasoning. *ICLR*, 2018.

Drew A. Hudson and Christopher D. Manning. Learning by abstraction: The neural state machine. In *NeurIPS*, 2019.

Huaizu Jiang, Xiaojian Ma, Weili Nie, Zhiding Yu, Yuke Zhu, and Anima Anandkumar. Bongard-hoi: Benchmarking few-shot visual reasoning for human-object interactions. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 19056–19065, 2022.

Daniel Keysers, Nathanael Schärli, Nathan Scales, Hylke Buisman, Daniel Furrer, Sergii Kashubin, Nikola Momchev, Danila Sinopalnikov, Lukasz Stafiniak, Tibor Tihon, et al. Measuring compositional generalization: A comprehensive method on realistic data. *International Conference on Learning Representations*, 2020.

Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

A. Krizhevsky. Learning multiple layers of features from tiny images. 2009.

Brenden M Lake, Ruslan Salakhutdinov, and Joshua B Tenenbaum. Human-level concept learning through probabilistic program induction. *Science*, 350(6266):1332–1338, 2015.

Brenden M Lake, Tomer D Ullman, Joshua B Tenenbaum, and Samuel J Gershman. Building machines that learn and think like people. *Behavioral and brain sciences*, 40, 2017.

Yann LeCun, Corinna Cortes, and CJ Burges. Mnist handwritten digit database. *ATT Labs [Online]. Available: http://yann.lecun.com/exdb/mnist*, 2, 2010.

Christoph von der Malsburg. The correlation theory of brain function. In *Models of neural networks*, pages 95–119. Springer, 1994.

Nikhil Mishra, Mostafa Rohaninejad, Xi Chen, and Pieter Abbeel. A simple neural attentive meta-learner. *arXiv preprint arXiv:1707.03141*, 2017.

Melanie Mitchell. Abstraction and analogy-making in artificial intelligence. *Annals of the New York Academy of Sciences*, 1505(1):79–101, 2021.

Yuval Netzer, Tao Wang, Adam Coates, Alessandro Bissacco, Bo Wu, and Andrew Y Ng. Reading digits in natural images with unsupervised feature learning. 2011.

Weili Nie, Zhiding Yu, Lei Mao, Ankit B Patel, Yuke Zhu, and Anima Anandkumar. Bongard-logo: A new benchmark for human-level concept learning and reasoning. *Advances in Neural Information Processing Systems*, 33:16468–16480, 2020.

Giambattista Parascandolo, Niki Kilbertus, Mateo Rojas-Carulla, and Bernhard Schölkopf. Learning independent causal mechanisms. In *International Conference on Machine Learning*, pages 4036–4044. PMLR, 2018.

Kha Pham, Hung Le, Man Ngo, and Truyen Tran. Functional indirection neural estimator for better out-of-distribution generalization. *NeurIPS*, 2022.

Nasim Rahaman, Muhammad Waleed Gondal, Shruti Joshi, Peter Gehler, Yoshua Bengio, Francesco Locatello, and Bernhard Schölkopf. Dynamic inference with neural interpreters. *Advances in Neural Information Processing Systems*, 34:10985–10998, 2021.

Murray Shanahan, Kyriacos Nikiforou, Antonia Creswell, Christos Kaplanis, David Barrett, and Marta Garnelo. An explicitly relational neural network architecture. In *International Conference on Machine Learning*, pages 8593–8603. PMLR, 2020.

Peter Shaw, Jakob Uszkoreit, and Ashish Vaswani. Self-attention with relative position representations. *arXiv preprint arXiv:1803.02155*, 2018.

Jake Snell, Kevin Swersky, and Richard Zemel. Prototypical networks for few-shot learning. *Advances in neural information processing systems*, 30, 2017.

Livio Baldini Soares, Nicholas FitzGerald, Jeffrey Ling, and Tom Kwiatkowski. Matching the blanks: Distributional similarity for relation learning. *arXiv preprint arXiv:1906.03158*, 2019.

Flood Sung, Yongxin Yang, Li Zhang, Tao Xiang, Philip HS Torr, and Timothy M Hospedales. Learning to compare: Relation network for few-shot learning. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 1199–1208, 2018.

Amos Tversky. Features of similarity. *Psychological review*, 84(4):327, 1977.

Ashish Vaswani, Noam M. Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. Attention is all you need. *NeurIPS*, abs/1706.03762, 2017.

Taylor Webb, Zachary Dulberg, Steven Frankland, Alexander Petrov, Randall O'Reilly, and Jonathan Cohen. Learning representations that support extrapolation. In *International conference on machine learning*, pages 10136–10146. PMLR, 2020a.

Taylor Whittington Webb, Ishan Sinha, and Jonathan Cohen. Emergent symbols through binding in external memory. In *International Conference on Learning Representations*, 2020b.

Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, Ed Chi, Quoc Le, and Denny Zhou. Chain of thought prompting elicits reasoning in large language models. *arXiv preprint arXiv:2201.11903*, 2022.

Chi Zhang, Feng Gao, Baoxiong Jia, Yixin Zhu, and Song-Chun Zhu. Raven: A dataset for relational and analogical visual reasoning. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, 2019.

APPENDIX

A DEFINITION OF $\hat{\delta}_\square$

We first define the rectangle distance $d_\square$ between graphs with the same set of vertices.

Definition A.1. (Borgs et al., 2008) Given two graphs $G = (V, E) \in \mathcal{G}_k$ and $G' = (V, E') \in \mathcal{G}_k$ with associated adjacency matrices $A_G = (a_{ij})_{i,j=\overline{1,k}}$ and $A_{G'} = (a'_{ij})_{i,j=\overline{1,k}}$. The *rectangle distance* $d_\square$ between G and G' is

$$d_\square(G, G') = \max_{S,T \subset V} \frac{1}{k^2} |e_G(S,T) - e_{G'}(S,T)|, \tag{4}$$

where

$$e_G(S,T) = \sum_{i \in S, j \in T} a_{ij} \quad \text{and} \quad e_{G'}(S,T) = \sum_{i \in S, j \in T} a'_{ij}.$$

The distance $d_\square$ can also be interpreted as the distance between the internal relationships (i.e., the adjacency matrices) of two graphs. However, one drawback of $d_\square$ is that it is not invariant under isomorphism. The generalized rectangle distance $\hat{\delta}_\square$ is proposed to overcome this drawback.

Definition A.2. (Borgs et al., 2008) Given two graphs $G = (V, E) \in \mathcal{G}_k$ and $G' = (V, E') \in \mathcal{G}_k$ with associated adjacency matrices $A_G = (a_{ij})_{i,j=\overline{1,k}}$ and $A_{G'} = (a'_{ij})_{i,j=\overline{1,k}}$. The *generalized rectangle distance* $\hat{\delta}_\square$ between G and G' is computed as $\hat{\delta}_\square(G, G') = \min_{\tilde{G} \cong G} d_\square(\tilde{G}, G')$, where $\tilde{G}$ shares the same set of vertices with G'.

B PROOFS OF THEORETICAL RESULTS

In this section, we provide proofs for theoretical results in the main text. An illustration of theoretical results are given in Fig. 4.

Proof of Theorem 3.2. Denote $\varepsilon = \hat{\delta}_\square(G, G')$. Since $G \cong f(G)$ and $G' \cong f(G')$, it folows that $\hat{\delta}_\square(f(G), f(G')) = \hat{\delta}_\square(G, G') = \varepsilon$. From the definition of $\hat{\delta}_\square$, there exists $G^{\text{ind}} \in \mathcal{G}_k^{\text{ind}}$ so that $G^{\text{ind}} \cong f(G)$ and $d_\square(G^{\text{ind}}, f(G')) = \varepsilon$. Denote $\mathcal{E} = A_{G^{\text{ind}}} - A_{f(G')}$, where $A_{G^{\text{ind}}}$ and $A_{f(G')}$ are the adjacency matrices of G^{ind} and $f(G')$ respectively, it follows from the definition of $d_\square$ that $\|\mathcal{E}\|_\infty \leq k^2\varepsilon$. Finally, note that $A_{f(G')} = A_{G'}$, we have

$$\begin{aligned}
\|r_G - r_{G'}\|_\infty &= \|(A_G V^{\text{ind}} - A_{G'} V^{\text{ind}}\|_\infty \\
&\leq \|A_G - A_{G^{\text{ind}}} + \mathcal{E}\|_\infty \|V^{\text{ind}}\|_\infty \\
&= \|A_{f(G)} - A_{G^{\text{ind}}} + \mathcal{E}\|_\infty \|V^{\text{ind}}\|_\infty \\
&\leq (\|A_G\|_\infty + \|A_{G^{\text{ind}}}\|_\infty + \|\mathcal{E}\|_\infty) \|V^{\text{ind}}\|_\infty \\
&\leq (2 + k^2\varepsilon)\|V^{\text{ind}}\|_\infty . \square
\end{aligned}$$

Proof of Theorem 3.3. Denote $[G] = \{\tilde{G} \in \mathcal{G}_k : \tilde{G} \cong G\}$. We will prove that for every $G_1 \in [G]$, there exits $G_2 \in [G']$ so that $\|r_{G_1} - r_{G_2}\|_\infty \leq k^2 \|V^{\text{ind}}\|_\infty \hat{\delta}(G, G')$.

Following the definition of $\hat{\delta}_\square$, for $G_1 \in [G]$, there exists $G_2 \in [G']$ so that $\hat{\delta}_\square(G_1, G') = d_\square(G_1, G_2)$. On the other hand, since $G_1 \cong G$, it follows that $\hat{\delta}_\square(G_1, G') = \hat{\delta}_\square(G, G')$, and hence $d_\square(G_1, G_2) = \hat{\delta}_\square(G, G')$. This leads to

$$\begin{aligned}
\|r_{G_1} - r_{G_2}\|_\infty &= \|A_{G_1} V^{\text{ind}} - A_{G_2} V^{\text{ind}}\|_\infty \\
&\leq \|A_{G_1} - A_{G_2}\|_\infty \|V^{\text{ind}}\|_\infty \\
&\leq k^2 d_\square(G_1, G_2) \|V^{\text{ind}}\|_\infty \\
&= k^2 \hat{\delta}_\square(G, G') \|V^{\text{ind}}\|_\infty .
\end{aligned}$$

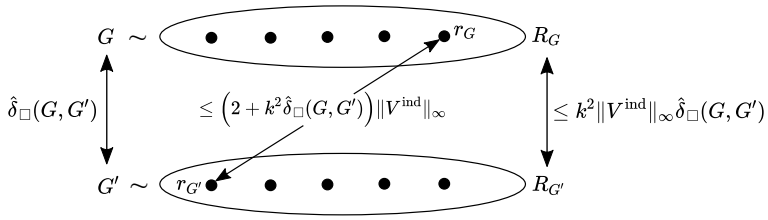


Figure 4: Illustration of Theorem 3.2 and Theorem 3.3.

This means

$$d(r_{G_1}, R_{G'}) = \inf_{\tilde{G}\in[G']} \|r_{G_1} - r_{\tilde{G}}\| \leq k^2\hat{\delta}_\square(G, G')\|V^{\text{ind}}\|_\infty$$

for every $G_1 \in [G]$. Similary, $d(r_{G_2}, R_G) = \inf_{\tilde{G}\in[G]} \|r_{G_2} - r_{\tilde{G}}\| \leq k^2\hat{\delta}_\square(G, G')\|V^{\text{ind}}\|_\infty$ for every $G_2 \in [G']$. This leads to

$$d_H(R_G, R_{G'}) = \max\left\{\sup_{G_1\in[G]} d(r_{G_1}, R_{G'}), \sup_{G_2\in[G']} d(r_{G_2}, R_G)\right\} \leq k^2\|V^{\text{ind}}\|_\infty\hat{\delta}(G, G').$$

Finally, if rank $V^{\text{ind}} = k$ and G and G' are not isomorphic, suppose there exists $r \in R_G \cap R_{G'}$. Since $r \in R_G$, there exists $G_1 \in [G]$ so that $r = r_{G_1} = A_{G_1}V^{\text{ind}}$. Similarly, there exists $G_2 \in [G']$ so that $r = A_{G_2}V^{\text{ind}}$. This leads to $A_{G_1}V^{\text{ind}} = A_{G_2}V^{\text{ind}}$, and since rank $V^{\text{ind}} = k$, we obtain $A_{G_1} = A_{G_2}$. This means $G_1 \cong G_2$, and hence $G \cong G'$, which is a contradiction. Hence $R_G \cap R_{G'} = \varnothing$. $\square$

C Full Experimental Results

C.1 OOD IQ Problems

C.1.1 FINE Dataset

We report full results with standard deviations of experiments on FINE dataset with trainset CIFAR10 and testset Omniglot in Table 5.

Train set Test set	CIFAR100 Omniglot			
	Trans.	Rot.	Shear	Scale
NTM	25.5±1.7/**56.9±5.0**	27.1±0.6/**31.4±1.7**	29.8±1.3/**58.5±4.6**	30.3±2.9/**61.0±3.9**
PrediNet	26.7±0.9/**28.5±4.5**	25.5±0.3/**28.3±0.5**	25.6±0.4/**29.0±1.7**	26.4±1.0/**29.9±1.7**
RelationNet	25.4±0.5/**39.3±1.4**	25.0±0.5/**34.0±0.4**	25.1±0.2/**39.8±1.1**	24.7±0.6/**50.2±1.0**
Transformer	26.9±1.9/**63.3±3.7**	27.2±1.1/**40.4±4.3**	28.3±1.4/**65.3±2.8**	30.6±3.0/**62.0±6.2**

Table 5: Test accuracy (%) without/with InLay on FINE dataset with trainset CIFAR10 and testset Omniglot.

We report full results with standard deviations of experiments on FINE dataset with trainset MNIST and testset CIFAR10 in Table 6.

Train set Test set	MNIST CIFAR100			
	Trans.	Rot.	Shear	Scale
NTM	35.2±1.6/**69.2±3.8**	30.0±1.9/**34.5±5.6**	29.6±1.1/**56.0±7.4**	31.9±4.7/**48.7±7.8**
PrediNet	27.5±1.4/**31.6±5.1**	26.8±1.4/**27.8±1.5**	26.4±1.4/**28.4±2.3**	33.6±2.5/**35.9±6.7**
RelationNet	25.6±0.5/**45.5±2.5**	25.6±0.6/**35.2±1.2**	25.0±0.5/**43.4±1.8**	26.8±0.7/**44.8±4.1**
Transformer	37.8±2.7/**63.9±6.5**	32.0±1.5/**36.1±10.1**	30.2±2.5/**53.5±6.8**	29.2±3.6/**48.1±7.0**

Table 6: Test accuracy (%) without/with InLay on FINE dataset.

C.1.2 RAVEN Dataset

We report full results with standard deviations of experiments on RAVEN dataset in Table 7.

Train configuration Test configuration	Up-Down Left-Right	3x3Grid 2x2Grid	Out-InGrid Out-InCenter
LSTM	28.8±3.1/**43.9±6.2**	19.5±0.6/**25.1±2.4**	42.1±1.3/**48.6±2.7**
Transformer	15.2±0.3/**56.7±2.3**	13.6±0.4/**26.0±0.9**	16.6±4.5/**44.7±1.6**
RelationNet	12.7±0.3/**58.5±2.0**	12.4±0.4/**28.9±0.4**	12.3±0.3/**51.7±2.8**
PrediNet	13.7±0.3/**16.5±0.9**	13.6±0.3/**14.3±0.6**	14.2±0.6/**15.9±0.5**

Table 7: Test accuracy (%) without/with InLay on RAVEN dataset.

C.2 OOD Image Classification

We report full results with standard deviations of OOD image classification experiments in Table 8.

Dataset	Image transformation		Color transformation			
	Rot90	VFlip	Jitter	Invert	Blur	Grayscale
SVHN	**16.4±0.5**/15.8±1.0	34.1±0.1/**35.3±0.5**	85.7±0.6/**90.2±0.2**	85.7±0.9/**90.1±0.3**	86.4±0.4/**89.8±1.0**	86.9±0.5/**91.8±0.7**
CIFAR10	25.7±0.1/**27.9±0.3**	32.1±0.6/**35.0±0.9**	23.2±1.1/**24.9±0.7**	39.4±2.8/**48.3±3.3**	**60.2±0.5**/59.5±1.2	48.3±0.8/**62.7±0.2**
CIFAR100	13.4±0.4/**15.0±0.2**	13.5±0.2/**16.8±0.5**	6.6±0.4/**9.7±0.3**	19.4±1.4/**23.4±2.2**	33.4±0.7/**33.5±1.0**	16.4±0.3/**23.9±0.4**

Table 8: Test accuracy (%) without/with InLay on OOD classification task with ViT.

C.3 Few-shot NLP Domain Adaptation

We report full results with standard deviations of few-shot NLP classification tasks on FewRel 2.0 dataset in Table 9.

	ProtoNet	SNAIL	GNN	MTB
5-way-1-shot	64.7±1.5/**65.4±3.0**	38.6±2.9/**60.6±4.9**	36.7±2.9/**63.1±1.3**	66.1±1.7/**68.9±1.0**
10-way-1-shot	**49.1±2.0**/41.7±3.2	17.3±1.2/**34.9±5.8**	27.1/**43.3±3.4**	52.9±1.2/**54.1±1.3**

Table 9: Validation accuracy (%) without/with InLay on FewRel 2.0.

D 6-layer ViT vs. 7-layer ViT

We report results of 6-layer ViT and 7-layer ViT, along with 6-layer ViT equipped with InLay, in OOD CIFAR10 classification tasks in Table 10. Overall, average performance of 6-layer ViT and 7-layer ViT is not much different (38.2% and 38%, respectively), while 6-layer ViT equipped with InLay clearly improve performances with average accuracy of 43.1%.

E Training Details

E.1 IQ OOD Problems

E.1.1 FINE Dataset

We use 3-layer $p4$-CNN encoder (Cohen and Welling, 2016) with kernel size 3 and padding 1 to encode raw 32×32 images to feature vectors of size 128. This encoder can help model adapt better with transformed images. We use Adam optimizer (Kingma and Ba, 2014) with learning rates ranging from 10^{-5} to $3 \cdot 10^{-4}$, depending on specific model and transformation. We train all models with batch size 32 in 200 epochs. The indirection representations are computed as in Eq. (1) with 1 attention head.

The training set contains 5,000 IQ problems, while testing set contains 10,000 IQ problems of unseen images and unseen rules. Specifically:

- With translation, models are trained on problems with translation vectors (a, b) with $a \in \{0, 3, 6, 9\}$ and $b \in \{0, \pm 3, \pm 6, \pm 9\}$, and tested with $a \in \{-3, -6, -9\}$, i.e., train on problems with translations to the right and test on problems with translations to the left.
- With rotation, models are trained on problems with rotation angle $\alpha \in \{0°, 15°, 30°, \ldots, 180°\}$, tested with $\alpha \in \{195°, 210°, \ldots, 345°\}$.

	Image transformation		Color transformation				Average
	Rot90	VFlip	Jitter	Invert	Blur	Grayscale	
6-layer ViT	25.7±0.1	32.1±0.6	23.2±1.1	39.4±2.8	60.2±0.5	48.3±0.8	38.2
7-layer ViT	26.4 ±0.5	31.5±0.3	22.4±1.2	38.6±3.2	**60.8 ±0.6**	48.3 ±0.7	38
6-layer ViT + InLay	**27.9±0.3**	**35.0±0.9**	**24.9±0.7**	**48.3±3.3**	59.5±1.2	**62.7±0.2**	**43.1**

Table 10: Test accuracy (%) without/with InLay on OOD CIFAR10 classification tasks with 6-layer ViT, 7-layer ViT, and 6-layer ViT equipped with InLay.

- With shear, models are trained on problems with shear angles (α, β) with $\alpha \in \{0, 15°, 30°, 45°, 60°\}$ and $\beta \in \{0, \pm 15°, \pm 30°, \pm 45°, \pm 60°\}$, and tested with $\alpha \in \{-15°, -30°, -45°, -60°\}$.
- With scale, models are trained on problems with scale factor $\alpha \in \{1, 1.25\}$ and tested with $\alpha \in \{0.5, 0.75\}$, i.e., train with larger scale and test with smaller scale.

E.1.2 RAVEN DATASET

We use 3-layer CNN encoder with kernel size 3 and stride 2 to encode 80×80 images to feature vectors of size 256. We use Adam optimizer with learning rates ranging from 10^{-4} to $3 \cdot 10^{-4}$ and gradient clipping 1. All models are trained with batch size 32 in 250 epochs. The indirection representations are computed as in Eq. (1) with 1 attention head.

We apply the Dynamic Residual Tree (DRT) as follows: we first apply DRT to feature vectors, then pass resulting vectors through InLay to obtain indirection representations, then apply DRT once again and these final resulting vectors will be the input for prediction models. Other details are similar to the original paper and codes are also adapted from the original paper.

E.2 OOD IMAGE CLASSIFICATION

We use Adam optimizer with learning rate $5 \cdot 10^{-4}$. All models are trained with batch size 32 in 200 epochs. The indirection representations are computed as in Eq. (1) with 32 attention heads.

We use 6-layer ViT with patch size 8, 16 attention heads and dropout rate 0.1. The dimension of feedforward layer is 2048.

E.3 FEW-SHOT NLP DOMAIN ADAPTATION

We use BERT to encode paragraphs to feature vectors of size 768. Models are trained with batch size 32 on 5-way-1-shot tasks and batch size 16 on 10-way-1-shot tasks. We use SGD optimizer with learning rate $2 \cdot 10^{-5}$. The indirection representations are computed as in Eq. (1) with 32 attention heads. Other details are similar to the original paper and codes are also adapted from the original paper.