GEOCON: COMPOSITIONAL GENERALIZATION THROUGH GEOMETRIC CONSTRAINTS ON REPRESENTATION STRUCTURE

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ABSTRACT

Compositional generalization, referring to the capacity to generalize novel combinations of fundamental and essential concepts, is thought to be the mechanism underlying a human's remarkable ability of rapid generalization to new knowledge and tasks. Recent research on brain neural activation space has found that the geometric structure of neural representations is highly related to human compositional generalization capability. In this paper, we extend the above observations from neuroscience to deep neural networks to validate the potential relationship between the geometric structure of representations and compositional generalization capability. In particular, we first construct a new compositional generalization benchmark, which aims to discriminate multiple concepts simultaneously through a powerful representation. Meanwhile, for the aforementioned geometric constraint, the parallelism score is formally defined for deep neural networks. Subsequently, we decompose the deep neural network into two parts: the featurizer and the classifier, to investigate the relationship between compositional generalization capability and parallelism score separately. Our proposed method, **Geo**metric **Con**straint (GeoCon), involves distance variance minimization regularization on the classifier and parallelism score maximization on the featurizer. Experiments on synthetic and real-world datasets demonstrate significant improvement of our approach, verifying the effectiveness of our neuroscience-inspired GeoCon approach towards human-like superior generalization ability.

1 INTRODUCTION

Humans exhibit a remarkable capacity for generalization by transferring existing limited prior knowledge to novel contexts. One underlying mechanism is hypothesized to be compositional generalization (Cole et al., 2013; Frankland & Greene, 2020; Hupkes et al., 2020), the ability to systematically disentangle learned concepts and recombine them into unseen compositions (e.g., *red apple* and *yellow banana* can be decoupled and recomposed into a new composition *yellow apple*). This ability, described by Chomsky (2014) as "the infinite use of finite means", is considered an essential characteristic of human intelligence. Despite the substantial advancements accomplished by deep neural networks (Li et al., 2021; Han et al., 2022), they still struggle with generalization performance and have been criticized for lacking compositional generalization capability, even when provided with extensive training data (Zhang et al., 2023). Consequently, it is a significant yet challenging research topic to study the compositional generalization mechanism of deep neural networks (Lin et al., 2023), which is crucial for advancing toward artificial intelligence.

Related Work. In previous research on compositional generalization in computer vision, one important related research field is disentangled representation learning (Higgins et al., 2017; Wang et al., 2022), which aims to extract independent underlying concept factors from mixed representations and recombine them to generate novel concept compositions predominantly on synthetic datasets. However, there is currently no evidence that explicitly decoupling input compositional factors substantially improves the learning efficiency or generalization capacity of models (Montero et al., 2020; Schott et al., 2021; Xu et al., 2022). Compositional zero-shot learning attempts to address the compositionality challenge in real-world scenarios, enhancing the accuracy of unseen attribute-object pairs when trained on different attribute-object pairs (Mancini et al., 2021; Wang

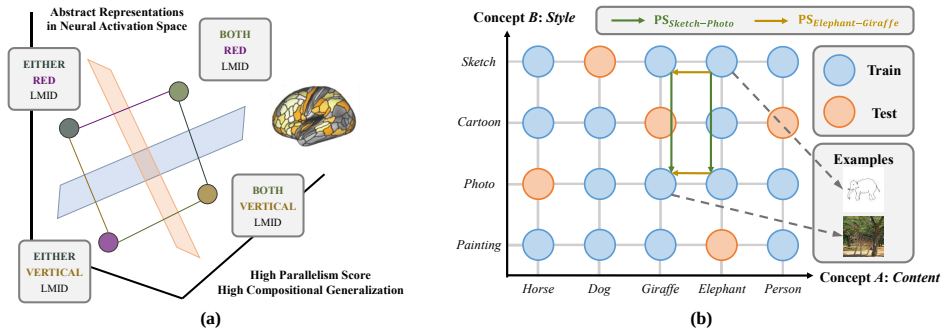

Figure 1: (a). Hypothetical geometric configurations of neural activation space. Parallel abstract representation leads to high compositional generalization capability. (b). Our designed compositional generalization benchmark. The model is expected to simultaneously differentiate two concepts.

et al., 2023; Hao et al., 2023). The objective of this task is to acquire invariant representations of objects while eliminating spurious attribute features, rather than systematically recognizing each concept, including attributes and objects. With the advancement of vision-language models (Zhang et al., 2024), several efforts have evaluated the compositional generalization capability of multimodal models (Ma et al., 2023; Yuksekgonul et al., 2023) and endeavored to develop novel training paradigms to enhance this ability (Zheng et al., 2024; Mitra et al., 2024). However, these purported improvements have been revealed to stem from linguistic priors rather than genuine enhancements in visual compositional generalization capability (Wu et al., 2023). Furthermore, extant visual encoders still perform inadequately in capturing compositional details (Tong et al., 2024). In summary, the internal mechanism of compositional generalization in visual models remains elusive.

To demystify the mechanism of compositional generalization from a neuroscience perspective, Bernardi et al. (2020) investigates the neural activation space in the hippocampus and prefrontal cortex, proposing the compositional additive representation extracted from neural signals, identified as the abstract representation. They further propose the parallelism score to quantify the parallelism of the geometric structure for the abstract representation, which is positively related to the compositional generalization capability, as shown in Fig.1.(a). The subsequent study (Ito et al., 2022) leverages the parallelism score to measure the fMRI activity signals of the human brain during the execution of tasks that necessitate logical decision, semantic comprehension, and motor response.

Our Contributions. Motivated by the aforementioned observations from neuroscience research, we would like to validate whether this pattern is consistent in deep neural networks. Initially, we establish a new benchmark for a compositional generalization task and provide a formal definition of the parallelism score. Afterwards, we partition the deep neural network into the featurizer and the classifier, proposing regularization techniques: distance variance minimization on the classifier and parallelism score maximization on the feature extractor, to constrain the representation space. As a result, we introduce the **Geo**metric **Con**straint (GeoCon) to strengthen the visual compositional generalization capability. Empirical studies demonstrate that our GeoCon method surpasses the current baselines across multiple datasets. This research endeavor has the potential to serve as a valuable investigation into the mechanisms underlying compositional generalization, thereby advancing the development of deep neural networks toward achieving human-like intelligence.

2 Preliminaries

2.1 Compositional Generalization

To achieve compositional generalization, it is imperative to systematically differentiate each concept and preserve the discrimination capacity for novel combinations. To facilitate comprehension and maintain simplicity, we shall initially examine the case of two concept factors, A and B. This framework can subsequently be expanded to encompass additional concepts.

Consider predicting the target $\boldsymbol{a} = (a_1, a_2, \ldots, a_{m_A}) \in \mathbb{R}^{m_A}$ with m_A concepts and target $\boldsymbol{b} = (b_1, b_2, \ldots, b_{m_B}) \in \mathbb{R}^{m_B}$ with m_B concepts simultaneously from input image $\boldsymbol{x} \in \mathbb{R}^{L \times H \times C}$.

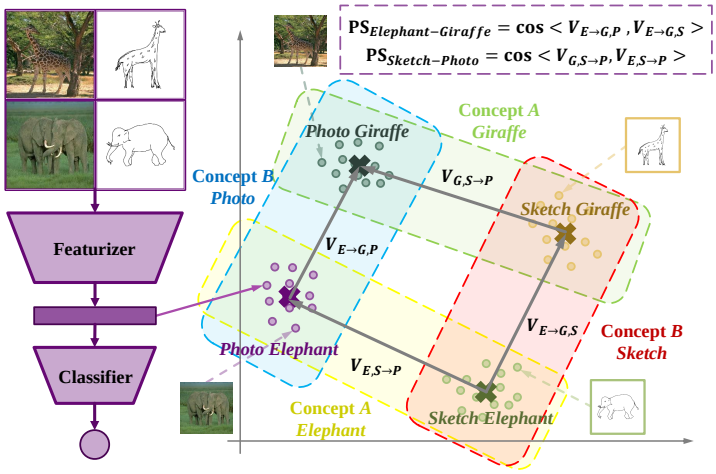

Figure 2: Illustration for the parallelism score calculation. We first calculate the expected representation for each combination, then obtain the concept transform vectors within diverse conceptual contexts (e.g., $\boldsymbol{V}_{E\to G,P}$ represents the concept transform vector that changes one concept from *Elephant* to *Giraffe* in the setting of *Photo* for another concept). Finally, we measure the parallelism of these concept transform vectors using the cosine similarity.

Featurizer can be defined as $g : \mathbb{R}^{L\times H\times C} \mapsto \mathbb{R}^d$ that maps an input image $\boldsymbol{x}$ into the d-dimensional representation space, while classifiers can be characterized as $f_A : \mathbb{R}^d \mapsto \mathbb{R}^{m_A}$ and $f_B : \mathbb{R}^d \mapsto \mathbb{R}^{m_B}$ that map a representation $\boldsymbol{r} = g(\boldsymbol{x})$ into A and B concept space respectively. The objective of this task is to develop the model $f_A \circ g$ and $f_B \circ g$ capable of accurately predicting multiple target concepts simultaneously, utilizing representations extracted by a single featurizer. In particular, to verify that g captures a good representation, we consider f_A and f_B to be the linear function to eschew further modifications of the representation structure.

Let $\mathcal{X}$ denote a nonempty input image space, as well as $\mathcal{A}$ and $\mathcal{B}$ two target spaces of concepts A and B. In the training process, we have training points $\mathcal{D}_{tr} = \{(\boldsymbol{x}^{(i)}, \boldsymbol{a}^{(i)}, \boldsymbol{b}^{(i)})\}_{i=1}^n$ sampled from distribution $\mathcal{D} = \mathcal{X} \times \mathcal{A} \times \mathcal{B}$. In the in-distribution generalization, the train set targets encompass all compositions within the concept space. However, in the compositional generalization setting, as demonstrated in Fig.1.(b), the train set targets will encounter each potential concept individually (containing all *styles* and *contents*), but there will still exist unseen concept combinations, which can be formally elucidated as:

$$\exists\, i \in \{1, 2, \ldots, m_A\}, j \in \{1, 2, \ldots, m_B\} \quad \text{s.t. } a_i \in \mathcal{A}_{tr}, b_j \in \mathcal{B}_{tr}, (a_i, b_j) \notin (\mathcal{A}_{tr} \times \mathcal{B}_{tr}) \tag{1}$$

where $\mathcal{A}_{tr}$ and $\mathcal{B}_{tr}$ denotes the training target spaces. The leftover space $(\mathcal{A}_{te} \times \mathcal{B}_{te}) = (\mathcal{A} \times \mathcal{B}) \setminus (\mathcal{A}_{tr} \times \mathcal{B}_{tr})$ is identified as the out-of-combination (OOC) in the target space. An ideal model exhibiting high compositional generalization capability can effectively learn from samples that only cover partial concept compositions but perform proficiency in OOC cases $\mathcal{D}_{te} = \mathcal{X}_{te} \times \mathcal{A}_{te} \times \mathcal{B}_{te}$, which characterize the test set, $\mathcal{X}_{te}$ denoting the corresponding input image space for $\mathcal{A}_{te} \times \mathcal{B}_{te}$.

Let $\mathcal{L}_{\mathcal{A}}(f_A, g; \mathcal{D}_{tr})$ and $\mathcal{L}_{\mathcal{B}}(f_B, g; \mathcal{D}_{tr})$ be cross-entropy loss functions that measures the discrepancy between the predictions and the targets, respectively. Accordingly, the compositional generalization can be formulated as the following optimization problem:

$$\min_{f_A, f_B, g} \mathbb{E}_{(\boldsymbol{x},\boldsymbol{a},\boldsymbol{b})\in\mathcal{D}_{tr}} \Big[\mathcal{L}_{\mathcal{A}}\big(f_A \circ g(\boldsymbol{x}), \boldsymbol{a}\big) + \mathcal{L}_{\mathcal{B}}\big(f_B \circ g(\boldsymbol{x}), \boldsymbol{b}\big) \Big] \tag{2}$$

2.2 Parallelism Score

We here provide a mathematical description for the parallelism score (PS) proposed qualitatively in neuroscience by Bernardi et al. (2020). Assign $\mathcal{X}(a, b) = \{\boldsymbol{x} \mid (\boldsymbol{x}, \boldsymbol{a}, \boldsymbol{b}) \in \mathcal{D}, (\boldsymbol{a}, \boldsymbol{b}) = (a, b)\}$ as the input samples with the target (a, b). Subsequently, we obtain the expected representation indicating the centroid for points with the target (a, b) as:

$$\overline{\boldsymbol{r}}(a, b) = \mathbb{E}_{\boldsymbol{x}\in\mathcal{X}(a,b)}[g(\boldsymbol{x})] \tag{3}$$

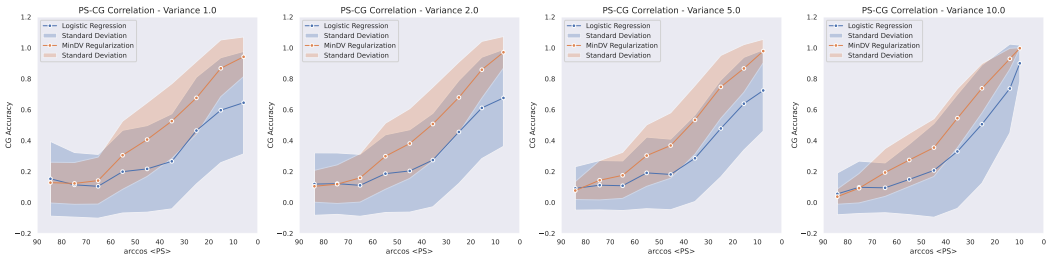

Figure 3: Positive correlation between PS and CG for logistic regression and MinDV regularization across the different variances for the Gaussian distributions. Since PS is nonlinear with respect to angle, the horizontal axis is converted to linear scale by the $\arccos$ function for clearer visualization.

Next, we introduce the concept transform vector of $a \to a'$ under context b, which measures the directional transformation of the expected representation of (a, b) to that of (a', b) as:

$$\boldsymbol{V}_{a\to a',b} = \boldsymbol{V}(a \to a'|b) = \overline{\boldsymbol{r}}(a', b) - \overline{\boldsymbol{r}}(a, b) \tag{4}$$

Correspondingly, the concept transform vector of $b \to b'$ under context a can be described as:

$$\boldsymbol{V}_{a,b\to b'} = \boldsymbol{V}(b \to b'|a) = \overline{\boldsymbol{r}}(a, b') - \overline{\boldsymbol{r}}(a, b) \tag{5}$$

The parallelism score (PS) intents to quantify the consistency of concept transform vector directions across diverse contexts, utilizing the cosine similarity function as a measurement, as illustrated in Fig.2. Consequently, it is feasible to define the specific-concept-level $\text{PS}_{a\to a'}$, the overall-concept-level PS_A, and the PS for the featurizer g with respect to set $\mathcal{D}$ as follows:

$$\text{PS}_{a\to a'} = \text{PS}(a \to a') = \frac{1}{M_B} \sum_{b\neq b' \in \mathcal{B}} \cos\left\langle \boldsymbol{V}(a \to a'|b), \boldsymbol{V}(a \to a'|b') \right\rangle \tag{6}$$

$$\text{PS}_A = \text{PS}(\boldsymbol{a}) = \frac{1}{M_A} \sum_{a\neq a' \in \mathcal{A}} \text{PS}(a \to a') \tag{7}$$

$$\text{PS}(g; \mathcal{D}) = \frac{M_A}{M_A + M_B}\text{PS}(\boldsymbol{a}) + \frac{M_B}{M_A + M_B}\text{PS}(\boldsymbol{b}) \tag{8}$$

where M_A is the quantity of pairs for $a \neq a'$ and M_B is the quantity of pairs for $b \neq b'$. The PS approaching 1 indicates highly parallel concept transform vectors, which may potentially lead to improved OOC performance, as suggested by Bernardi et al. (2020). This characteristic exhibits the potential to facilitate the training of models with enhanced compositional generalization capability.

3 METHODOLOGY

In this section, we aim to validate the effectiveness of the parallelism score (PS) from neuroscience on deep neural networks by investigating the correlation between PS and compositional generalization (CG) capability. Specifically, we partition the neural network into a featurizer that extracts representations and a classifier that makes final decisions based on these representations linearly. We seek to address the following inquiries: What kind of classifier can enhance robust CG capability? What kind of featurizer can yield high PS representations?

3.1 CLASSIFIER: DISTANCE VARIANCE MINIMIZATION

Simulation Studies on Synthetic Datasets. Assuming the existence of representations captured by the featurizer, we aim to explore the relationship between representation geometric structure and CG capability. Considering the simplest scenario involving two targets $\boldsymbol{a} = (a_1, a_2)$ and $\boldsymbol{b} = (b_1, b_2)$ with two-dimensional representations that can be visualized on a plane, on which we sample four points on a unit circle and consider them as centroids of representations with the concept combinations (a_1, b_1), (a_1, b_2), (a_2, b_1), and (a_2, b_2). By controlling the sampled points, we can manipulate the PS of the representation centroids. We further sample points around these centroids from the

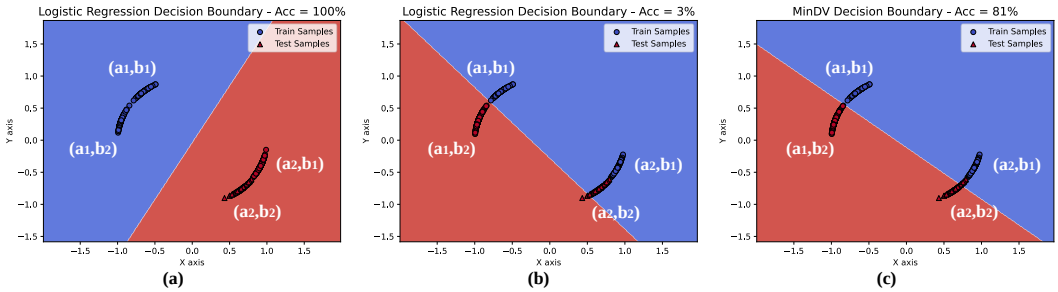

Figure 4: A fail case occurs when the PS of the sample points is 0.99. (a). Logistic regression exhibits 100% accuracy when classifying concepts a_1 and a_2. (b). Logistic regression has only 3% accuracy when classifying concepts b_1 and b_2. (c). After applying MinDV regularization, the accuracy improves to 81% when classifying concepts b_1 and b_2.

Gaussian distributions along the proximal circumference, to facilitate the generation of a synthetic dataset of representations with different PS, all retaining the same concept labels as the centroids.

Subsequently, the points centered at (a_2, b_2) are designated as the test set, while points centered at (a_1, b_1), (a_1, b_2) and (a_2, b_1) constitute the train set. We train two linear classifiers to classify $\boldsymbol{a} = (a_1, a_2)$ and $\boldsymbol{b} = (b_1, b_2)$. During the training process, the model is exposed to all concepts a_1, a_2, and b_1, b_2. Nevertheless, it has not encountered the combination of (a_2, b_2), which is defined as the out-of-combination for CG. The mean and standard deviation of the accuracy of simultaneously classifying the targets correctly within different PS intervals are recorded, as shown in Fig.3.

The blue line in Fig.3 illustrates the relationship between PS and CG when logistic regression is employed as the linear classifier. As the PS increases, the model's CG accuracy also improves, demonstrating a positive correlation. A higher PS suggests that the configuration of the centroids more closely approximates a parallelogram rather than an irregular quadrilateral, resulting in greater parallelism between edges and making it more feasible for the model to accomplish CG tasks. The blue shaded area represents the variance in accuracy, a larger variance implies instability in CG accuracy. This observation suggests that even when the representations exhibit high PS, the model retains a significant probability of demonstrating poor CG capability.

We conduct a detailed analysis of cases where CG fails under high PS representations. In Fig.4.(a), when classifying concepts a_1 and a_2, the distance between them is significant, allowing for distinct classification. However, a severe failure occurs when classifying concepts b_1 and b_2 with an accuracy of only 3%, as depicted in Fig.4.(b). During the training process, the logistic regression model tends to maximize the aggregate distances from all train sample points (circle points) to the decision boundary. Nevertheless, while classifying (a_2, b_1) and (a_2, b_2), since the test sample points (triangle points) centered around (a_2, b_2) are unseen, the model will attempt to make the decision boundary as far away as possible from the visible (a_2, b_1)-centered points (meanwhile getting closer to the unseen (a_2, b_2)-centered points), in order to achieve enhanced basic generalization (albeit at the expense of the CG capability). To address the aforementioned challenges, we propose distance variance minimization regularization on the classifier to enhance the CG capability.

Distance Variance Minimization. The vanilla classifier demonstrates a failure on out-of-combination samples, due to neglecting the highly parallel geometric structures of representations. In this case, we aim for all samples to have as similar distances to the decision boundary as possible, essentially minimizing the variance of distances. This strategy can prevent the model from deviating excessively from the (a_2, b_2)-center points, based on which we propose **D**istance **V**ariance **Min**imization (MinDV) regularization to achieve this insight.

In more detail, when f is a linear function, defined as $f(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{r} + \boldsymbol{b}$, where $\boldsymbol{r} = g(\boldsymbol{x})$, we know that the distance between the point and the decision boundary is $|\boldsymbol{w}^T \boldsymbol{r} + \boldsymbol{b}| / \|\boldsymbol{w}\|_2$. The distance variance (DV) of the samples from the decision boundary on dataset $\mathcal{D}$ can be denoted as:

$$\mathrm{DV}(f, g; \mathcal{D}) = \mathrm{Var}_{\boldsymbol{x} \in \mathcal{X}} \left[\frac{|\boldsymbol{w}^T g(\boldsymbol{x}) + \boldsymbol{b}|}{\|\boldsymbol{w}\|_2} \right] \tag{9}$$

Smaller DV indicates that the decision boundary is more parallel to the concept transform vectors.

Ideally, we aim to solve the following constrained optimization problem. If this objective is feasible, then our solution can rectify the failures. We generalize this finding in the subsequent theorem.

$$\begin{aligned} &\min_{f_A, f_B, g} \mathbb{E}_{(\boldsymbol{x},\boldsymbol{a},\boldsymbol{b})\in\mathcal{D}_{tr}}\Big[\mathcal{L}_{\mathcal{A}}(f_A, g; \mathcal{D}_{tr}) + \mathcal{L}_{\mathcal{B}}(f_B, g; \mathcal{D}_{tr})\Big] \\ &\text{s.t.} \quad \mathrm{DV}(f_A, g; \mathcal{D}_{tr}) = 0,\ \mathrm{DV}(f_B, g; \mathcal{D}_{tr}) = 0 \end{aligned} \tag{10}$$

Theorem 1. *If we do not consider the stochastic noise of the feature distribution, assume that PS $= 1$, and the representation space is linearly separable, then f calculated by Eq.10 is guaranteed to have 100% accuracy, while vanilla classifier may fail for some cases.*

Provided that DV $= 0$ is extremely challenging in practice, we relax the formulation constraint to:

$$\begin{aligned} &\min_{f_A, f_B, g} \mathbb{E}_{(\boldsymbol{x},\boldsymbol{a},\boldsymbol{b})\in\mathcal{D}_{tr}}\Big[\mathcal{L}_{\mathcal{A}}(f_A, g; \mathcal{D}_{tr}) + \mathcal{L}_{\mathcal{B}}(f_B, g; \mathcal{D}_{tr})\Big] \\ &\text{s.t.} \quad \mathrm{DV}(f_A, g; \mathcal{D}_{tr}) \leq \epsilon,\ \mathrm{DV}(f_B, g; \mathcal{D}_{tr}) \leq \epsilon \end{aligned} \tag{11}$$

where ϵ is the tolerance coefficient. The above is equivalent to the Lagrange function with appropriate hyperparameters α_A and α_B, where the last terms are identified as the MinDV regularization:

$$\min_{f_A, f_B, g} \mathbb{E}\Big[\mathcal{L}_{\mathcal{A}}(f_A, g; \mathcal{D}_{tr}) + \mathcal{L}_{\mathcal{B}}(f_B, g; \mathcal{D}_{tr})\Big] + \alpha_A \mathrm{DV}(f_A, g; \mathcal{D}_{tr}) + \alpha_B \mathrm{DV}(f_B, g; \mathcal{D}_{tr}) \tag{12}$$

The MinDV regularization promotes model consistency in the distance from the decision boundary across all samples. The idea of "balance enhances generalization" has also been applied in domain generalization. For instance, the Invariant Risk Minimization (IRM) (Arjovsky et al., 2019) algorithm aims to achieve similar classification performance across diverse domains while maintaining overall classification efficacy. In summary, both MinDV and IRM are based on the assumption that there exists a substantial disparity between the observed training distribution and the unseen testing distribution. They strive to ensure that the model performs similarly across all visible distributions, rather than significantly outperforming on a specific distribution.

After utilizing MinDV, the previously failed case is rectified effectively, with performance improving from 3% to 81%, as shown in Fig.4.(c). Moreover, the orange line in Fig.3 depicts the results after incorporating MinDV. Concomitant with the increase in CG accuracy, the variance is effectively controlled, indicating a reduction in the quantity of failed cases. Overall, there exists a strong positive correlation between PS and CG, with higher PS expected to yield better CG performance.

3.2 Featurizer: Parallelism Score Maximization

Empirical Studies on Real-world Datasets. To explore what characteristic of the models can achieve high PS representations, we evaluate multiple pre-trained models on the PACS, Office-Home and NICO datasets for PS and CG capabilities, also validating whether the above conclusions remain effective in more complex real-world scenarios. In specific, these datasets are broadly used in domain generalization, typically annotated with *class* and *domain* labels. We treat them as two target concepts and establish the CG tasks following Section 2.1. We select 65 pre-trained models with different architectures, sizes, training strategies, and training datasets from the `timm` library (Wightman, 2019). Through freezing their featurizers' parameters and conducting linear probing solely on representations, we evaluate the CG capabilities.

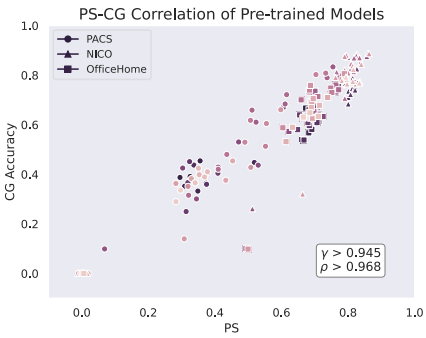

Figure 5: The $\mathrm{PS}_{\mathrm{class}}$ and $\mathrm{CG}_{\mathrm{class}}$ for different models across multiple datasets. Different colors represent different pre-trained models, different shapes represent different datasets.

We separately record the $\mathrm{PS}_{\mathrm{class}}$ and $\mathrm{PS}_{\mathrm{domain}}$, $\mathrm{CG}_{\mathrm{class}}$ and $\mathrm{CG}_{\mathrm{domain}}$, yielding the following insights:

(i). *A positive correlation exists between PS and CG, and this conclusion still holds true even in real-world environments*. As depicted in Fig.5, Pearson's correlation (γ) and Spearman's rank correlation (ρ) coefficient both exceed 0.945, further emphasizing this robust correlation irrespective of dataset variations.

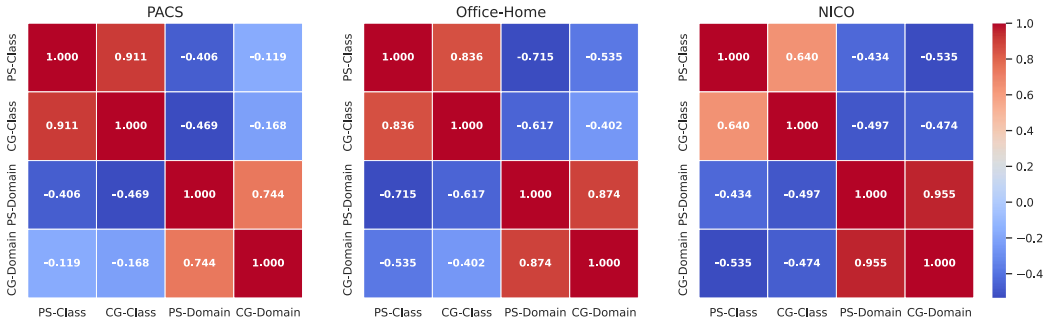

Figure 6: The Spearman correlation matrices of the PACS, Office-Home, and NICO datasets.

(ii). *Different models exhibit varying PS and CG capabilities across different concepts.* As indicated by the blue region in Fig.6, the CG_{class} shows a negative correlation with the $\text{PS}_{\text{domain}}$ and $\text{CG}_{\text{domain}}$. This suggests that models with strong CG capabilities for *class* may have weaker CG capabilities for *domain*, indicating that the CG capabilities across different concepts are not necessarily correlated.

(iii). *The pre-training strategy of a model influences its PS and CG capability.* Models with randomly initialized weights inherently exhibit high PS for *domain*, showcasing the best $\text{CG}_{\text{domain}}$ performance but negligible CG_{class} capability. Compared to supervised models, the self-supervised model DINO demonstrates a balanced performance on both *class* and *domain*, potentially because supervised models excessively focus on the *class* during the pre-training phase. For supervised models, increasing the amount of training data or scaling up the model size can enhance the CG_{class} capability but does not improve the $\text{CG}_{\text{domain}}$ capability. Multimodal models like CLIP exhibit superior CG capabilities for both *class* and *domain*. Refer to the Appendix C for more details.

(iv). *Even the most advanced models struggle to exhibit strong CG capabilities across multiple concepts simultaneously.* So far, no model has demonstrated extremely strong CG capabilities in class or domain aspects. CG continues to be a highly complex and challenging task.

Parallelism Score Maximization. Existing models encounter difficulties in simultaneously possessing high PS across multiple concepts, thereby limiting their CG capabilities. Consequently, an intuitive approach is to utilize PS as a constraint and explicitly optimize it during the training process. Therefore, we propose the **P**arallelism **S**core **Max**imization (MaxPS) regularization, which encourages the representations to possess a highly parallel geometric structure. Since PS is a cosine function with an upper bound of 1, we achieve this by minimizing the difference between PS and 1.

Suppose that T denotes the number of iterations. At each $t = 1, \ldots, T$ round, we get a batch of stochastic samples $\mathcal{D}_{tr}^t = \mathcal{X}_{tr}^t \times \mathcal{A}_{tr}^t \times \mathcal{B}_{tr}^t$. Following the mathematical definition in Eq.3, initially, we estimate the expected representation using batch samples as:

$$\hat{\boldsymbol{r}}^t(a,b) = \mathbb{E}_{\boldsymbol{x} \in \mathcal{X}_{tr}^t(a,b)}[g(\boldsymbol{x})] \tag{13}$$

When the batch size is large enough, this estimation approximates the actual expected value. If the batch size is limited, we can also employ an exponential smoothing method (Cutkosky & Orabona, 2019) to reduce the variance. According to Eq.8, the estimations of PS can be calculated as follows:

$$\begin{aligned}\hat{\text{PS}}(g_t; \mathcal{D}_{tr}^t) = \frac{1}{M_A^t + M_B^t} \sum_{a \neq a' \in \mathcal{A}_{tr}^t} \sum_{b \neq b' \in \mathcal{B}_{tr}^t} \Big(& \frac{1}{M_B^t} \cos\big\langle \hat{\boldsymbol{V}}^t(a \to a'|b), \hat{\boldsymbol{V}}^t(a \to a'|b') \big\rangle \\ & + \frac{1}{M_A^t} \cos\big\langle \hat{\boldsymbol{V}}^t(b \to b'|a), \hat{\boldsymbol{V}}^t(b \to b'|a') \big\rangle \Big)\end{aligned} \tag{14}$$

where $\hat{\boldsymbol{V}}^t(a \to a'|b) = \hat{\boldsymbol{r}}^t(a,b) - \hat{\boldsymbol{r}}^t(a',b)$. Under the assumption of uniformly sampled concept transform vectors, this estimation can be proved unbiased as follows.

Theorem 2. *Assume that the concept transform vectors are uniformly sampled, and* $\hat{\boldsymbol{r}}^t(a,b) \approx \overline{\boldsymbol{r}}(a,b)$*, we have:* $\mathbb{E}[\hat{PS}(g_t; \mathcal{D}_{tr}^t)] \approx PS(g; \mathcal{D}_{tr})$.

Theorem 2 indicates that PS can be appropriately optimized. One might argue that uniformly sampled concept transform vectors may be too strong. In practice, we can reweight each pair of concept transform vectors to ensure equal influence, thereby potentially obtaining equivalent results.

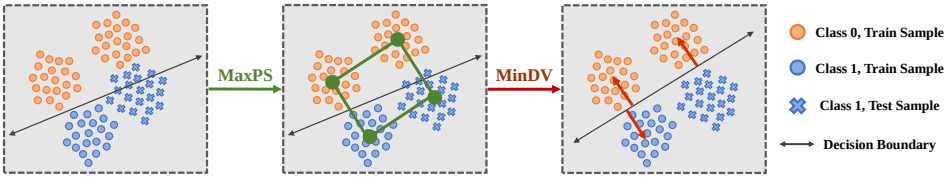

Figure 7: The Geometric Constraint framework.

By leveraging the PS estimation, we get the MaxPS regularized loss for the batch t as:

$$\tilde{\mathcal{L}}_t = \mathcal{L}_{\mathcal{A}}(f_A^t, g_t; \mathcal{D}_{tr}^t) + \mathcal{L}_{\mathcal{B}}(f_B^t, g_t; \mathcal{D}_{tr}^t) + \beta(1 - \hat{\text{PS}}(g_t; \mathcal{D}_{tr}^t)) \tag{15}$$

and then perform gradient steps for descending $\tilde{\mathcal{L}}_t$ to update the model and obtain f_A^{t+1}, f_B^{t+1} and g_{t+1} until the parameter converges. The MaxPS regularization ensures that the representation models are enforced to optimize the accuracy and PS simultaneously, leading to better CG performance.

3.3 Framework: Geometric Constraint

Based on the positive correlation between PS and CG capability, we introduce two regularizations: MinDV primarily constrains the geometric structure of the classifier, whereas MaxPS imposes constraints on the the representations extracted by the featurizer. By combining Eq.12 and Eq.15, we propose the **Geo**metric **Con**straint (GeoCon) method to enhance CG capability via PS and DV:

$$\min_{f_A, f_B, g} \mathbb{E}\Big[\mathcal{L}_{\mathcal{A}}(f_A, g) + \mathcal{L}_{\mathcal{B}}(f_B, g)\Big] + \alpha_A \hat{\text{DV}}(f_A, g) + \alpha_B \hat{\text{DV}}(f_B, g) + \beta(1 - \hat{\text{PS}}(g)) \tag{16}$$

where α_A, α_B and β denote the weights of the regularization terms. Fig.7 illustrates the workflow of GeoCon, where MaxPS encourages more parallelism among the centroids of the representations, while MinDV ensures a more equitable distribution of distances between sample points and decision boundary, thus conforming to this well-organized geometric structure. Refer to the Appendix A for the proof of the theorem and the Appendix B for detailed optimization steps.

4 Experiments

4.1 Setup

Datasets. As described in Section 2.1, the CG benchmark requires each sample to have at least two concept labels. Therefore, domain generalization datasets that concurrently annotate *class* and *domain* labels would serve as an feasible solution. We select the **PACS** (Li et al., 2017), **Office-Home** (Saenko et al., 2010), **DomainNet** (Peng et al., 2019), and **NICO** (He et al., 2021) datasets, considering their *class* and *domain* labels as two separate concepts, to construct our CG benchmark, among which PACS, Office-Home, and DomainNet have concepts labeled as *content* and *style*, while NICO's concepts are labeled as *object* and *environment*.

Due to the significant disparity in the quantity of *classes* compared to *domains* in the Office-Home, DomainNet, and NICO datasets, there exists a substantial difficulty gap between classifying the two targets. To address this issue, we divide the datasets by *class* into several subsets, each containing a comparable number of *classes* as the number of *domains*, and record the average performance across these subsets. For each *class*, one *domain* is selected as the test set, while the remaining *domains* serve as the train set, ensuring that all *domains* have appeared in the train set.

For deeper analysis, we additionally leverage the synthetic dataset **3D Shapes** (Kim & Mnih, 2018), composed of 6 factors: *floor hue*, *wall hue*, *object hue*, *scale*, *shape*, and *orientation*. We identify *shape* and *object hue* as the concepts to be predicted, while regarding the other factors as noise, providing a reasonable simulation of the real world. We randomly sample 1000 images for each concept combination to construct our dataset. Half of the concept combinations are used for training, while the remaining combinations are employed for testing. Each image is flattened into a one-dimensional vector, and a three-layer fully connected neural network is employed, wherein the first two layers are shared by two concepts, serving as a featurizer. Subsequently, two linear classifiers are connected to classify *shape* and *object hue*, respectively.

Table 1: CG accuracy of models with different pre-training settings. Bold indicates the best result.

Dataset		PACS			Office-Home			DomainNet			NICO		
Backbone	Method	class	domain	both	class	domain	both	class	domain	both	class	domain	both
ViT_{1K}	LP	0.4083	0.6834	0.2195	0.9155	0.2732	0.0789	0.3548	0.6052	0.1769	0.9313	0.2008	0.1521
	FT	0.7307	0.6655	0.4060	0.9127	0.3499	0.1553	0.7098	0.6125	0.3534	0.9323	0.2472	0.2366
	GeoCon	0.7896	0.6938	**0.4804**	0.9324	0.3962	**0.2513**	0.7103	0.6523	**0.4352**	0.9416	0.3228	**0.3071**
ViT_{21K}	LP	0.5614	0.8433	0.4197	0.9465	0.2113	0.1690	0.5120	0.7513	0.3589	0.9550	0.3358	0.3047
	FT	0.7197	0.9085	0.6317	0.9437	0.2535	0.2000	0.6988	0.8230	0.5584	0.9629	0.3534	0.3233
	GeoCon	0.7884	0.9521	**0.7409**	0.9606	0.3299	**0.2965**	0.7765	0.8425	**0.6327**	0.9643	0.4420	**0.4151**
DINO	LP	0.4609	0.8245	0.2976	0.8366	0.2901	0.1549	0.4327	0.7450	0.2520	0.9323	0.3131	0.2630
	FT	0.5206	0.8245	0.3536	0.8394	0.3296	0.1775	0.4888	0.7552	0.3052	0.9341	0.3298	0.2782
	GeoCon	0.5493	0.8449	**0.4043**	0.8451	0.4231	**0.2780**	0.5075	0.8012	**0.3721**	0.8562	0.4212	**0.3344**
CLIP	LP	0.9384	0.9262	0.8645	0.9155	0.462	0.3831	0.9012	0.8532	0.7865	0.9699	0.3984	0.3766
	FT	0.9234	0.9623	0.8857	0.9324	0.5803	0.5155	0.9026	0.8781	0.8014	0.9689	0.3789	0.3534
	GeoCon	0.9713	0.9910	**0.9623**	0.9014	0.6563	**0.5775**	0.9155	0.9352	**0.8552**	0.9768	0.4940	**0.4819**

Table 2: Comparison for CG accuracy of different methods on CLIP. Bold indicates the best result.

Dataset	PACS			Office-Home			DomainNet			NICO			**Average**
Method	class	domain	both	class	domain	both	class	domain	both	class	domain	both	both
LP	0.9384	0.9262	0.8645	0.9155	0.4620	0.3831	0.9012	0.8532	0.7865	0.9699	0.3984	0.3766	0.6027
FT	0.9234	0.9623	0.8857	0.9324	0.5803	0.5155	0.9026	0.8781	0.8014	0.9689	0.3789	0.3534	0.6390
LP-FT	0.9352	0.9713	0.9066	0.9218	0.6064	0.5216	0.9058	0.8810	0.8021	0.9702	0.3884	0.3615	0.6480
WiSE-FT	0.9399	0.9706	0.9109	0.9201	0.6255	0.5520	0.9094	0.9053	0.8233	0.9703	0.4402	0.4151	0.6753
GeoCon w/o MaxPS	0.9431	0.9761	0.9195	0.9147	0.6028	0.5433	0.9137	0.9184	0.8401	0.9712	0.4671	0.4439	0.6867
GeoCon w/o MinDV	0.9368	0.9623	0.8991	0.9195	0.6312	0.5524	0.9121	0.9136	0.8345	0.9717	0.4893	0.4763	0.6906
GeoCon	**0.9713**	**0.9910**	**0.9623**	**0.9114**	**0.6563**	**0.5775**	**0.9155**	**0.9352**	**0.8552**	**0.9768**	**0.4940**	**0.4819**	**0.7192**

Baselines. We implement the classifiers of the two concepts as single-layer linear classifiers. For the featurizer, we employ a ViT-Base-16 architecture and select models from the `timm` library (Wightman, 2019) under different training settings, including: $\mathbf{ViT_{1K}}$ (supervised training on ImageNet 1K), $\mathbf{ViT_{21K}}$ (supervised training on ImageNet 21K), **DINO** (self-supervised training) (Oquab et al., 2023), and **CLIP** (contrastive language-image pre-training) (Radford et al., 2021). CLIP tuning is an important research problem in transfer learning. To further validate the effectiveness of our approach, we select linear probing (**LP**), fine-tuning (**FT**), **LP-FT** (Kumar et al., 2022), and **WiSE-FT** (Wortsman et al., 2022) as baselines for comparison, where LP-FT does LP first and then FT after some epochs, WiSE-FT uses a weighted average of parameters before and after FT.

4.2 Main Results

Tab.1 presents the *class* accuracy, *domain* accuracy, and both accuracy (classifying two concepts accurately simultaneously) on multiple datasets when utilizing pre-trained models under different training settings. Irrespective of the backbone employed, our method consistently demonstrates remarkably superior performance, thus substantiating the effectiveness of our approach. ViT_{21K}, compared to ViT_{1K}, demonstrates enhanced CG capability due to the increased training data volume. The supervised ViT_{1K} and ViT_{21K} result in higher performance in *class* accuracy, whereas the self-supervised DINO shows a more balanced performance in *class* accuracy and *domain* accuracy. CLIP continues to serve as a robust featurizer for CG tasks, surpassing other backbones significantly.

Tab.2 further analyzes the results of different algorithms when using CLIP as the backbone. Although WiSE-FT serves as a strong baseline for out-of-distribution generalization, our method still achieves state-of-the-art performance in this task. LP-FT shows a marginal improvement compared to LP and FT, suggesting that conventional methods focusing solely on train set accuracy may just enhance basic generalization but struggle to achieve strong CG capability. Furthermore, we conduct ablation studies to elucidate the importance of each component in our GeoCon framework. The results indicate that even independently utilizing one single component can lead to optimal performance. In comparison, MaxPS may be more critical since it primarily influences the featurizers with more parameters. In addition, an observation reveals the presence of a "Buckets Effect" in CG tasks, wherein the both accuracy is more susceptible to concepts that are difficult to discriminate.

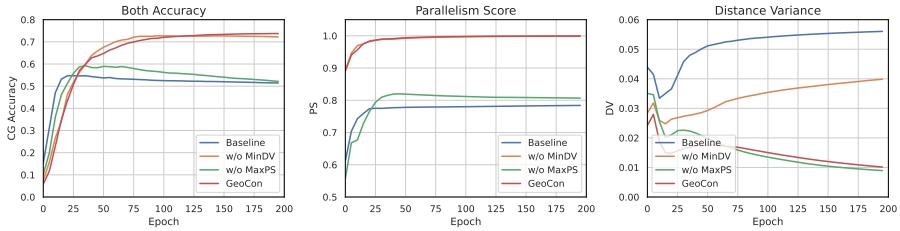

Figure 8: The training process on 3D Shapes Dataset.

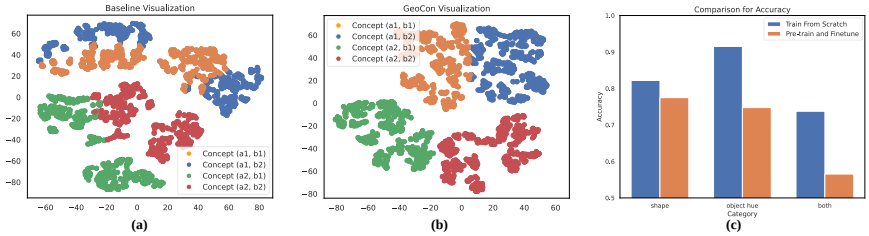

Figure 9: (a). t-SNE visualization when using baseline method. (b). t-SNE visualization when using GeoCon framework. (c). Comparison of the accuracy with (blue) and without (orange) pre-training.

4.3 Discussions

We conduct a more comprehensive analysis on the 3D Shapes dataset, leveraging supervised learning without the addition of any regularization as the baseline model. Fig.8 illustrates the variation of metrics during the training process, wherein our approach demonstrates a significant improvement of 22.29% compared to the baseline. When MaxPS is not used, the model converges rapidly but experiences a decrease in accuracy after 25 epochs. It is noteworthy that the improvement in accuracy aligns precisely with the uplift of PS, while the decline in accuracy corresponds to the stagnation of PS. Maintaining consistency with MaxPS, the application of MinDV leads to lower DV and improved accuracy, without which DV will ascend.

Fig.9.(a) and (b) display the t-SNE visualization results. The representations from the baseline model still tend to cluster together but exhibit poor separability. In contrast, our GeoCon method produces highly separable representations characterized by distinct linear discriminability.

To investigate the impact of pre-training on CG, we initially train a featurizer supervised by *shape* solely and subsequently fine-tune it according to the CG setting. Surprisingly, the pre-trained models demonstrated lower accuracy compared to models trained from scratch, as depicted in Fig.9.(c). This could be attributed to biases introduced during the pre-training phase that are challenging to entirely eliminate during fine-tuning. This observation suggests that simply fine-tuning existing pre-trained models may not be efficacious for enhancing CG performance. The development of algorithms with stronger CG capability necessitates consideration from the pre-training stage.

5 Conclusions

Conclusions. We formally introduce the parallelism score from neuroscience to deep learning, revealing a strong positive correlation between it and compositional generalization from a geometry perspective. Our framework, GeoCon, consisting of MinDV for the classifier and MaxPS for the featurizer, aims to enhance CG capability by constraining the geometric structures of representations and forcing the decision boundaries to conform to the well-organized structure. Experiments show that GeoCon outperforms traditional approaches. This neuroscience-inspired representation mechanism may elucidate the fundamental nature of human-like intelligence in deep neural networks.

Limitations. Our GeoCon currently relies on aligned concepts, presenting challenges when scaling up to more complex and productive tasks. Furthermore, the computation of PS requires a substantial quantity of concept combinations inside each batch, which is of relative inefficiency. This issue could potentially be addressed by introducing a memory bank to mitigate computational complexity.

REFERENCES

Martin Arjovsky, Léon Bottou, Ishaan Gulrajani, and David Lopez-Paz. Invariant risk minimization. *arXiv preprint arXiv:1907.02893*, 2019.

Silvia Bernardi, Marcus K Benna, Mattia Rigotti, Jérôme Munuera, Stefano Fusi, and C Daniel Salzman. The geometry of abstraction in the hippocampus and prefrontal cortex. *Cell*, 183(4): 954–967, 2020.

Noam Chomsky. *Aspects of the Theory of Syntax*. Number 11. 2014.

Michael W Cole, Patryk Laurent, and Andrea Stocco. Rapid instructed task learning: A new window into the human brain's unique capacity for flexible cognitive control. *Cognitive, Affective, & Behavioral Neuroscience*, 13:1–22, 2013.

Ashok Cutkosky and Francesco Orabona. Momentum-based variance reduction in non-convex sgd. *Advances in neural information processing systems*, 32, 2019.

Steven M Frankland and Joshua D Greene. Concepts and compositionality: in search of the brain's language of thought. *Annual review of psychology*, 71(1):273–303, 2020.

Kai Han, Yunhe Wang, Hanting Chen, Xinghao Chen, Jianyuan Guo, Zhenhua Liu, Yehui Tang, An Xiao, Chunjing Xu, Yixing Xu, et al. A survey on vision transformer. *IEEE transactions on pattern analysis and machine intelligence*, 45(1):87–110, 2022.

Shaozhe Hao, Kai Han, and Kwan-Yee K Wong. Learning attention as disentangler for compositional zero-shot learning. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 15315–15324, 2023.

Yue He, Zheyan Shen, and Peng Cui. Towards non-iid image classification: A dataset and baselines. *Pattern Recognition*, 110:107383, 2021.

Irina Higgins, Loic Matthey, Arka Pal, Christopher P Burgess, Xavier Glorot, Matthew M Botvinick, Shakir Mohamed, and Alexander Lerchner. beta-vae: Learning basic visual concepts with a constrained variational framework. *ICLR (Poster)*, 3, 2017.

Dieuwke Hupkes, Verna Dankers, Mathijs Mul, and Elia Bruni. Compositionality decomposed: How do neural networks generalise? *Journal of Artificial Intelligence Research*, 67:757–795, 2020.

Takuya Ito, Tim Klinger, Doug Schultz, John Murray, Michael Cole, and Mattia Rigotti. Compositional generalization through abstract representations in human and artificial neural networks. *Advances in neural information processing systems*, 35:32225–32239, 2022.

Hyunjik Kim and Andriy Mnih. Disentangling by factorising. In *International conference on machine learning*, pp. 2649–2658. PMLR, 2018.

Ananya Kumar, Aditi Raghunathan, Robbie Jones, Tengyu Ma, and Percy Liang. Fine-tuning can distort pretrained features and underperform out-of-distribution. *arXiv preprint arXiv:2202.10054*, 2022.

Da Li, Yongxin Yang, Yi-Zhe Song, and Timothy M Hospedales. Deeper, broader and artier domain generalization. In *Proceedings of the IEEE international conference on computer vision*, pp. 5542–5550, 2017.

Zewen Li, Fan Liu, Wenjie Yang, Shouheng Peng, and Jun Zhou. A survey of convolutional neural networks: analysis, applications, and prospects. *IEEE transactions on neural networks and learning systems*, 2021.

Baihan Lin, Djallel Bouneffouf, and Irina Rish. A survey on compositional generalization in applications. *arXiv preprint arXiv:2302.01067*, 2023.

Zixian Ma, Jerry Hong, Mustafa Omer Gul, Mona Gandhi, Irena Gao, and Ranjay Krishna. Crepe: Can vision-language foundation models reason compositionally? In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 10910–10921, 2023.

Massimiliano Mancini, Muhammad Ferjad Naeem, Yongqin Xian, and Zeynep Akata. Open world compositional zero-shot learning. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 5222–5230, 2021.

Chancharik Mitra, Brandon Huang, Trevor Darrell, and Roei Herzig. Compositional chain-of-thought prompting for large multimodal models. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 14420–14431, 2024.

Milton Llera Montero, Casimir JH Ludwig, Rui Ponte Costa, Gaurav Malhotra, and Jeffrey Bowers. The role of disentanglement in generalisation. In *International Conference on Learning Representations*, 2020.

Maxime Oquab, Timothée Darcet, Théo Moutakanni, Huy Vo, Marc Szafraniec, Vasil Khalidov, Pierre Fernandez, Daniel Haziza, Francisco Massa, Alaaeldin El-Nouby, et al. Dinov2: Learning robust visual features without supervision. *arXiv preprint arXiv:2304.07193*, 2023.

Xingchao Peng, Qinxun Bai, Xide Xia, Zijun Huang, Kate Saenko, and Bo Wang. Moment matching for multi-source domain adaptation. In *Proceedings of the IEEE/CVF international conference on computer vision*, pp. 1406–1415, 2019.

Alec Radford, Jong Wook Kim, Chris Hallacy, Aditya Ramesh, Gabriel Goh, Sandhini Agarwal, Girish Sastry, Amanda Askell, Pamela Mishkin, Jack Clark, et al. Learning transferable visual models from natural language supervision. In *International conference on machine learning*, pp. 8748–8763. PMLR, 2021.

Kate Saenko, Brian Kulis, Mario Fritz, and Trevor Darrell. Adapting visual category models to new domains. In *Computer Vision–ECCV 2010: 11th European Conference on Computer Vision, Heraklion, Crete, Greece, September 5-11, 2010, Proceedings, Part IV 11*, pp. 213–226. Springer, 2010.

Lukas Schott, Julius Von Kügelgen, Frederik Träuble, Peter Gehler, Chris Russell, Matthias Bethge, Bernhard Schölkopf, Francesco Locatello, and Wieland Brendel. Visual representation learning does not generalize strongly within the same domain. *arXiv preprint arXiv:2107.08221*, 2021.

Shengbang Tong, Zhuang Liu, Yuexiang Zhai, Yi Ma, Yann LeCun, and Saining Xie. Eyes wide shut? exploring the visual shortcomings of multimodal llms. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 9568–9578, 2024.

Qingsheng Wang, Lingqiao Liu, Chenchen Jing, Hao Chen, Guoqiang Liang, Peng Wang, and Chunhua Shen. Learning conditional attributes for compositional zero-shot learning. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 11197–11206, 2023.

Xin Wang, Hong Chen, Si'ao Tang, Zihao Wu, and Wenwu Zhu. Disentangled representation learning. *arXiv preprint arXiv:2211.11695*, 2022.

Ross Wightman. Pytorch image models. `https://github.com/rwightman/pytorch-image-models`, 2019.

Mitchell Wortsman, Gabriel Ilharco, Jong Wook Kim, Mike Li, Simon Kornblith, Rebecca Roelofs, Raphael Gontijo Lopes, Hannaneh Hajishirzi, Ali Farhadi, Hongseok Namkoong, et al. Robust fine-tuning of zero-shot models. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 7959–7971, 2022.

Chenwei Wu, Li Erran Li, Stefano Ermon, Patrick Haffner, Rong Ge, and Zaiwei Zhang. The role of linguistic priors in measuring compositional generalization of vision-language models. In *Proceedings on*, pp. 118–126. PMLR, 2023.

Zhenlin Xu, Marc Niethammer, and Colin A Raffel. Compositional generalization in unsupervised compositional representation learning: A study on disentanglement and emergent language. *Advances in Neural Information Processing Systems*, 35:25074–25087, 2022.

Mert Yuksekgonul, Federico Bianchi, Pratyusha Kalluri, Dan Jurafsky, and James Zou. When and why vision-language models behave like bags-of-words, and what to do about it? In *The Eleventh International Conference on Learning Representations*, 2023.

Jingyi Zhang, Jiaxing Huang, Sheng Jin, and Shijian Lu. Vision-language models for vision tasks: A survey. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2024.

Le Zhang, Rabiul Awal, and Aishwarya Agrawal. Contrasting intra-modal and ranking cross-modal hard negatives to enhance visio-linguistic fine-grained understanding. *arXiv preprint arXiv:2306.08832*, 2023.

Chenhao Zheng, Jieyu Zhang, Aniruddha Kembhavi, and Ranjay Krishna. Iterated learning improves compositionality in large vision-language models. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 13785–13795, 2024.

A PROOF FOR THEOREM

A.1 PROOF FOR THEOREM 1

Proof. We shall begin with a 2-dimensional and 2-concept case. Assume that we have 4 points are (a_1, a_2), (b_1, b_2), (c_1, c_2), (d_1, d_2) with target (y_1, y_2), (y_1', y_2), (y_1, y_2'), (y_1', y_2'). If PS $= 1$, then we have:

$$\boldsymbol{V}_{y_1 \to y_1', y_2} = (b_1 - a_1, b_2 - a_2) = (d_1 - c_1, d_2 - c_2) = \boldsymbol{V}_{y_1 \to y_1', y_1}$$
$$\boldsymbol{V}_{y_1, y_2 \to y_2'} = (c_1 - a_1, c_2 - a_2) = (d_1 - b_1, d_2 - b_2) = \boldsymbol{V}_{y_1', y_2 \to y_2'}$$

Since the representation space is linearly separable, we can easily know that the optimal classifier (considering the whole combination cases, hence have the best CG performance) for separating y_1 and y_1' is:

$$y = \frac{c_2 - a_2}{c_1 - a_1}(x - \frac{a_1 + b_1}{2}) + \frac{a_2 + b_2}{2}$$

which is parallel to $\boldsymbol{V}_{y_1, y_2 \to y_2'}$ and $\boldsymbol{V}_{y_1', y_2 \to y_2'}$. And the optimal classifier for separating y_2 and y_2 is:

$$y = \frac{b_2 - a_2}{b_1 - a_1}(x - \frac{a_1 + c_1}{2}) + \frac{a_2 + c_2}{2}$$

which is parallel to $\boldsymbol{V}_{y_1, y_2 \to y_2'}$ and $\boldsymbol{V}_{y_1', y_2 \to y_2'}$.

Then, suppose the training points are (a_1, a_2), (b_1, b_2), (c_1, c_2), the optimal solution of Eq.10 is exactly the same with the above optimal classifier that performs 100% accuracy when classifying (d_1, d_2).

However, if four points are $A = (1, 1)$, $B = (2, 1)$, $C = (-1, 0)$, $D = (0, 0)$, then vanilla regression on A, B and C will have solution for separating y_2 and y_2:

$$x = \frac{3}{2}$$

which fail to classify D. We now prove that in the above case, Eq.10 yields a perfect model, while vanilla regression could fail.

In the more generalized case involving multiple concepts and higher dimensionality, the principle still comprises several instances of the 4-point cases. The generalization of our theoretical framework is readily achievable. □

A.2 PROOF FOR THEOREM 2

Proof. Since we know that $\hat{\boldsymbol{r}}^t(a,b) \approx \overline{\boldsymbol{r}}^t(a,b)$, we can get:

$$\hat{\boldsymbol{V}}^t_{a\to a',b} = \hat{\boldsymbol{r}}(a',b) - \hat{\boldsymbol{r}}(a,b) \approx \overline{\boldsymbol{r}}(a',b) - \overline{\boldsymbol{r}}(a,b) = \boldsymbol{V}^t_{a\to a',b},$$
$$\hat{\boldsymbol{V}}^t_{a,b\to b'} = \hat{\boldsymbol{r}}(a,b') - \hat{\boldsymbol{r}}(a,b) \approx \overline{\boldsymbol{r}}(a,b') - \overline{\boldsymbol{r}}(a,b) = \boldsymbol{V}^t_{a,b\to b'}.$$

For simplicity, we assume that $M_t = M^t_A = M^t_B$ in Eq.14 and $M = M_A = M_B$ in Eq.8. Due to the concept transform vectors are uniformly sampled, we have:

$$\begin{aligned}
\mathbb{E}[\hat{\mathrm{PS}}(g_t;\mathcal{D}^t_{tr})] &= \mathbb{E}\left[\frac{1}{2M_t^2}\sum_{a\neq a'\in\mathcal{A}^t_{tr}}\sum_{b\neq b'\in\mathcal{B}^t_{tr}}\left(\cos\left\langle\hat{\boldsymbol{V}}^t_{a\to a',b},\hat{\boldsymbol{V}}^t_{a\to a',b'}\right\rangle + \cos\left\langle\hat{\boldsymbol{V}}^t_{a,b\to b'},\hat{\boldsymbol{V}}^t_{a',b\to b'}\right\rangle\right)\right] \\
&\approx \mathbb{E}\left[\frac{1}{2M_t^2}\sum_{a\neq a'\in\mathcal{A}^t_{tr}}\sum_{b\neq b'\in\mathcal{B}^t_{tr}}\left(\cos\left\langle\boldsymbol{V}^t_{a\to a',b},\boldsymbol{V}^t_{a\to a',b'}\right\rangle + \cos\left\langle\boldsymbol{V}^t_{a,b\to b'},\boldsymbol{V}^t_{a',b\to b'}\right\rangle\right)\right] \\
&= \frac{1}{2M^2}\sum_{a\neq a'\in\mathcal{A}_{tr}}\sum_{b\neq b'\in\mathcal{B}_{tr}}\left(\cos\left\langle\boldsymbol{V}^t_{a\to a',b},\boldsymbol{V}^t_{a\to a',b'}\right\rangle + \cos\left\langle\boldsymbol{V}^t_{a,b\to b'},\boldsymbol{V}^t_{a',b\to b'}\right\rangle\right) \\
&= \mathrm{PS}(g;\mathcal{D}_{tr}).
\end{aligned}$$

We thus end the proof. □

B OPTIMIZATION STEPS FOR GEOCON

Algorithm 1 Geometric Constraint for Compositional Generalization

Input: training dataset $\mathcal{D}_{tr} = \{(\boldsymbol{x}^{(i)}, \boldsymbol{a}^{(i)}, \boldsymbol{b}^{(i)})\}_{i=1}^{N}$, batch size M, learning rate η, training steps T, regularization weights α_A, α_B, β
Output: featuizer g, classifier f_A for concept A, classifier f_B for concept B parameterized as θ
for $t = 1$ to T **do**
  get mini-batch data from $\mathcal{D}_{tr}$: $\mathcal{D}_{tr}^t = \{(\boldsymbol{x}^{(i)}, \boldsymbol{a}^{(i)}, \boldsymbol{b}^{(i)})\}_{i=1}^{M}$
  for $\forall (a, b) \in (\mathcal{A}_{tr}^t \times \mathcal{B}_{tr}^t)$ **do**
    calculate mean representations: $\hat{\boldsymbol{r}}^t(a, b)$ by Eq.3
  end for
  for $b = 1$ to $|\boldsymbol{b}|$ **do**
    for $\forall a \neq a' \in \mathcal{A}_{tr}^t$ **do**
      if $(a, b) \wedge (a', b) \in (\mathcal{A}_{tr}^t \times \mathcal{B}_{tr}^t)$ **then**
        calculate concept $a \to a'$ transform vectors: $\hat{\boldsymbol{V}}^t(a \to a'|b)$ by Eq.4
      end if
    end for
  end for
  for $a = 1$ to $|\boldsymbol{a}|$ **do**
    for $\forall b \neq b' \in \mathcal{B}_{tr}^t$ **do**
      if $(a, b) \wedge (a, b') \in (\mathcal{A}_{tr}^t \times \mathcal{B}_{tr}^t)$ **then**
        calculate concept $b \to b'$ transform vectors: $\hat{\boldsymbol{V}}^t(b \to b'|a)$ by Eq.5
      end if
    end for
  end for
  for $\forall a \neq a' \in \mathcal{A}_{tr}^t$ **do**
    for $\forall b \neq b' \in \mathcal{B}_{tr}^t$ **do**
      if $(a, b) \wedge (a, b') \wedge (a', b) \wedge (a', b') \in (\mathcal{A}_{tr}^t \times \mathcal{B}_{tr}^t)$ **then**
        calculate parallelism score: $\hat{\text{PS}}(g_t; \mathcal{D}_{tr}^t)$ by Eq.8
      end if
    end for
  end for
  for $i = 1$ to M **do**
    calculate distances: $\dfrac{\|f_A \circ g(\boldsymbol{x}^{(i)})\|}{\|\boldsymbol{w}_A\|_2}$ and $\dfrac{\|f_B \circ g(\boldsymbol{x}^{(i)})\|}{\|\boldsymbol{w}_B\|_2}$
    calculate cross-entropy loss: $\mathcal{L}_{\mathcal{A}}(f_A^t, g_t; \mathcal{D}_{tr}^t)$ and $\mathcal{L}_{\mathcal{B}}(f_B^t, g_t; \mathcal{D}_{tr}^t)$
  end for
  calculate distance variance: $\hat{\text{DV}}_A(f_A^t, g_t; \mathcal{D}_{tr}^t)$ and $\hat{\text{DV}}_B(f_B^t, g_t; \mathcal{D}_{tr}^t)$ by Eq.10
  calculate total loss: $\tilde{\mathcal{L}}_t = \mathcal{L}_{\mathcal{A}} + \mathcal{L}_{\mathcal{B}} + \alpha_A \hat{\text{DV}}_A + \alpha_B \hat{\text{DV}}_B + \beta(1 - \hat{\text{PS}})$ by Eq.16
  update parameters by stochastic gradient descent: $\theta_{t+1} \leftarrow \theta_t - \eta \dfrac{\partial \tilde{\mathcal{L}}_t}{\partial \theta_t}$
end for

C THE PS AND CG ACCURACY OF DIFFERENT PRE-TRAINED MODELS

Table 3: The PS and CG Accuracy of different pre-trained models on the PACS dataset.

Model	PS-class	CG-class	PS-domain	CG-domain
resnet18_random	-0.0017	0	0.9929	1
resnet18_tv_in1k	0.3697	0.3805	0.5864	0.8499
resnet18_fb_ssl_yfcc100m_ft_in1k	0.3951	0.3542	0.6127	0.8591
resnet18_fb_swsl_ig1b_ft_in1k	0.5225	0.5012	0.5724	0.8569
resnet34_tv_in1k	0.3581	0.4055	0.574	0.8533
resnet50_random	-0.0024	0	0.9946	1
resnet50_tv2_in1k	0.3354	0.4073	0.5663	0.8526
resnet50_fb_ssl_yfcc100m_ft_in1k	0.4263	0.3418	0.6004	0.8682
resnet50_fb_swsl_ig1b_ft_in1k	0.6123	0.6333	0.5608	0.8711
resnet101_tv2_in1k	0.3256	0.3844	0.5751	0.8206
resnet152_tv2_in1k	0.3325	0.383	0.563	0.812
wide_resnet50_2_tv2_in1k	0.3221	0.3	0.5606	0.8504
wide_resnet101_2_tv2_in1k	0.3171	0.4144	0.586	0.8411
vit_small_patch8_224_dino	0.4028	0.5302	0.6058	0.8552
vit_small_patch16_224_augreg_in1k	0.3432	0.3062	0.5409	0.8248
vit_small_patch16_224_augreg_in21k	0.4456	0.3945	0.6144	0.9193
vit_small_patch16_224_augreg_in21k_ft_in1k	0.4629	0.4464	0.5911	0.9064
vit_small_patch16_224_dino	0.3678	0.3412	0.627	0.8852
vit_small_patch32_224_augreg_in21k	0.3778	0.3477	0.5804	0.8894
vit_small_patch32_224_augreg_in21k_ft_in1k	0.3747	0.3717	0.5694	0.8434
vit_base_patch16_224_random	-0.0021	0	0.9493	1
vit_base_patch16_224_augreg_in1k	0.3813	0.3497	0.5481	0.8089
vit_base_patch16_224_augreg_in21k	0.4876	0.5275	0.6244	0.9364
vit_base_patch16_224_augreg_in21k_ft_in1k	0.5514	0.5543	0.572	0.8588
vit_base_patch16_224_dino	0.3854	0.3928	0.6108	0.8767
vit_base_patch16_224_mae	0.1319	0.132	0.5857	0.8246
vit_base_patch16_clip_224_laion2b	0.7491	0.8638	0.7334	0.9719
vit_base_patch16_clip_224_laion2b_ft_in1k	0.6145	0.6976	0.5328	0.8891
vit_base_patch16_clip_224_laion2b_ft_in12k_in1k	0.535	0.5601	0.4925	0.8523
vit_base_patch16_clip_224_openai	0.7369	0.8035	0.6761	0.9287
vit_base_patch16_clip_224_openai_ft_in1k	0.6225	0.7693	0.4733	0.8417
vit_base_patch16_clip_224_openai_ft_in12k_in1k	0.5292	0.6341	0.4515	0.833
vit_base_patch32_224_random	-0.0023	0	0.9443	1
vit_base_patch32_224_augreg_in1k	0.3447	0.281	0.5534	0.8168
vit_base_patch32_224_augreg_in21k	0.4187	0.4261	0.6191	0.8761
vit_base_patch32_224_augreg_in21k_ft_in1k	0.4432	0.4463	0.5786	0.8837
vit_base_patch32_clip_224_laion2b	0.7293	0.769	0.7193	0.9794
vit_base_patch32_clip_224_laion2b_ft_in12k_in1k	0.5185	0.5523	0.4712	0.8698
vit_base_patch32_clip_224_laion2b_ft_in1k	0.5537	0.5642	0.5367	0.8507
vit_large_patch16_224_random	-0.0017	0	0.9591	1
vit_large_patch16_224_augreg_in21k	0.519	0.514	0.6279	0.9267
vit_large_patch16_224_augreg_in21k_ft_in1k	0.6149	0.7023	0.5985	0.901
vit_large_patch16_224_mae	0.3074	0.1342	0.7857	0.9129

Table 4: The PS and CG Accuracy of different pre-trained models on the Office-Home dataset.

Model	PS-class	CG-class	PS-domain	CG-domain
resnet18_random	0.0161	0	0.9836	1
resnet18_tv_in1k	0.6987	0.5559	0.2555	0.5614
resnet18_fb_ssl_yfcc100m_ft_in1k	0.6864	0.5463	0.2697	0.5828
resnet18_fb_swsl_ig1b_ft_in1k	0.7135	0.5805	0.2755	0.562
resnet34_tv_in1k	0.7136	0.5832	0.2605	0.5532
resnet50_random	0.0052	0	0.9864	1
resnet50_tv2_in1k	0.6928	0.634	0.2068	0.5092
resnet50_fb_ssl_yfcc100m_ft_in1k	0.6997	0.6165	0.265	0.5774
resnet50_fb_swsl_ig1b_ft_in1k	0.7273	0.6706	0.2637	0.5846
resnet101_tv2_in1k	0.71	0.641	0.2266	0.4892
resnet152_tv2_in1k	0.7141	0.6467	0.2068	0.5004
wide_resnet50_2_tv2_in1k	0.6883	0.625	0.1963	0.5056
wide_resnet101_2_tv2_in1k	0.7085	0.6609	0.2115	0.4888
vit_small_patch8_224_dino	0.6678	0.594	0.3636	0.6542
vit_small_patch16_224_augreg_in1k	0.7231	0.6369	0.1632	0.5289
vit_small_patch16_224_augreg_in21k	0.7143	0.7102	0.2644	0.6167
vit_small_patch16_224_augreg_in21k_ft_in1k	0.7568	0.7141	0.2421	0.6003
vit_small_patch16_224_dino	0.6454	0.5095	0.3521	0.6715
vit_small_patch32_224_augreg_in21k	0.7115	0.6799	0.2402	0.5897
vit_small_patch32_224_augreg_in21k_ft_in1k	0.7378	0.6772	0.2182	0.5654
vit_base_patch16_224_random	0.0051	0	0.86	1
vit_base_patch16_224_augreg_in1k	0.7437	0.6238	0.1542	0.4942
vit_base_patch16_224_augreg_in21k	0.7019	0.7528	0.269	0.6549
vit_base_patch16_224_augreg_in21k_ft_in1k	0.7881	0.7672	0.2145	0.6212
vit_base_patch16_224_dino	0.6549	0.57	0.3472	0.6412
vit_base_patch16_224_mae	0.4166	0.097	0.32	0.5989
vit_base_patch16_clip_224_laion2b	0.7106	0.7438	0.4751	0.8177
vit_base_patch16_clip_224_laion2b_ft_in1k	0.8073	0.7896	0.1993	0.5451
vit_base_patch16_clip_224_laion2b_ft_in12k_in1k	0.7951	0.7867	0.1775	0.54
vit_base_patch16_clip_224_openai	0.7039	0.6471	0.4516	0.7672
vit_base_patch16_clip_224_openai_ft_in1k	0.7937	0.7489	0.1831	0.5408
vit_base_patch16_clip_224_openai_ft_in12k_in1k	0.784	0.7741	0.1441	0.4959
vit_base_patch32_224_random	0.0026	0	0.8676	1
vit_base_patch32_224_augreg_in1k	0.7135	0.6194	0.1566	0.5114
vit_base_patch32_224_augreg_in21k	0.677	0.6995	0.2499	0.6128
vit_base_patch32_224_augreg_in21k_ft_in1k	0.729	0.7089	0.2156	0.5676
vit_base_patch32_clip_224_laion2b	0.6972	0.7091	0.4539	0.7953
vit_base_patch32_clip_224_laion2b_ft_in12k_in1k	0.7721	0.7539	0.1671	0.5093
vit_base_patch32_clip_224_laion2b_ft_in1k	0.7741	0.7277	0.2166	0.5577
vit_large_patch16_224_random	0.0014	0	0.884	1
vit_large_patch16_224_augreg_in21k	0.7122	0.76	0.2768	0.6472
vit_large_patch16_224_augreg_in21k_ft_in1k	0.8136	0.7998	0.2303	0.61
vit_large_patch16_224_mae	0.5065	0.1118	0.4222	0.6601

Table 5: The PS and CG Accuracy of different pre-trained models on the NICO dataset.

Model	PS-class	CG-class	PS-domain	CG-domain
resnet18_random	-0.0054	0	0.9897	1
resnet18_tv_in1k	0.8006	0.6717	0.4011	0.4513
resnet18_fb_ssl_yfcc100m_ft_in1k	0.8051	0.7289	0.4053	0.4573
resnet18_fb_swsl_ig1b_ft_in1k	0.8109	0.7523	0.3912	0.4388
resnet34_tv_in1k	0.8113	0.7188	0.3819	0.4372
resnet50_random	-0.0045	0	0.9913	1
resnet50_tv2_in1k	0.8014	0.7859	0.3164	0.3652
resnet50_fb_ssl_yfcc100m_ft_in1k	0.8168	0.8115	0.3707	0.4154
resnet50_fb_swsl_ig1b_ft_in1k	0.826	0.8213	0.3603	0.4153
resnet101_tv2_in1k	0.7966	0.7756	0.3287	0.3609
resnet152_tv2_in1k	0.7946	0.7531	0.3271	0.3749
wide_resnet50_2_tv2_in1k	0.7996	0.7827	0.3005	0.3642
wide_resnet101_2_tv2_in1k	0.7961	0.7816	0.2914	0.3678
vit_small_patch8_224_dino	0.8159	0.8305	0.3382	0.4306
vit_small_patch16_224_augreg_in1k	0.8206	0.7719	0.2464	0.351
vit_small_patch16_224_augreg_in21k	0.8135	0.8385	0.4044	0.4613
vit_small_patch16_224_augreg_in21k_ft_in1k	0.8409	0.8418	0.3805	0.4273
vit_small_patch16_224_dino	0.782	0.7706	0.3601	0.4564
vit_small_patch32_224_augreg_in21k	0.79	0.7651	0.3861	0.4743
vit_small_patch32_224_augreg_in21k_ft_in1k	0.8109	0.7705	0.3657	0.4583
vit_base_patch16_224_random	-0.0018	0	0.9084	1
vit_base_patch16_224_augreg_in1k	0.8262	0.7621	0.238	0.3502
vit_base_patch16_224_augreg_in21k	0.7935	0.8639	0.3827	0.4567
vit_base_patch16_224_augreg_in21k_ft_in1k	0.8575	0.8711	0.363	0.4124
vit_base_patch16_224_dino	0.7989	0.7964	0.3495	0.436
vit_base_patch16_224_mae	0.6242	0.2528	0.7944	0.5234
vit_base_patch16_clip_224_laion2b	0.8265	0.8786	0.4397	0.4998
vit_base_patch16_clip_224_laion2b_ft_in1k	0.8258	0.8644	0.2296	0.3262
vit_base_patch16_clip_224_laion2b_ft_in12k_in1k	0.8269	0.8683	0.2171	0.3369
vit_base_patch16_clip_224_openai	0.8329	0.8653	0.4059	0.4673
vit_base_patch16_clip_224_openai_ft_in1k	0.8303	0.8641	0.1984	0.333
vit_base_patch16_clip_224_openai_ft_in12k_in1k	0.8219	0.877	0.2143	0.3453
vit_base_patch32_224_random	0.0038	0	0.9015	1
vit_base_patch32_224_augreg_in1k	0.7887	0.699	0.2814	0.4104
vit_base_patch32_224_augreg_in21k	0.7631	0.8044	0.384	0.4683
vit_base_patch32_224_augreg_in21k_ft_in1k	0.8088	0.8187	0.3572	0.4399
vit_base_patch32_clip_224_laion2b	0.8147	0.8384	0.4445	0.5143
vit_base_patch32_clip_224_laion2b_ft_in12k_in1k	0.8087	0.8475	0.2305	0.3434
vit_base_patch32_clip_224_laion2b_ft_in1k	0.7972	0.8231	0.2537	0.3618
vit_large_patch16_224_random	-0.0014	0	0.9192	1
vit_large_patch16_224_augreg_in21k	0.7883	0.8746	0.3744	0.476
vit_large_patch16_224_augreg_in21k_ft_in1k	0.8641	0.8838	0.3553	0.4164
vit_large_patch16_224_mae	0.6728	0.3345	0.5714	0.5421