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# Connecting Sphere Manifolds Hierarchically for Regularization

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## Abstract

This paper considers classification problems with hierarchically organized classes. We force the classifier (hyperplane) of each class to belong to a sphere manifold, whose center is the classifier of its super-class. Then, individual sphere manifolds are connected based on their hierarchical relations. Our technique replaces the last layer of a neural network by combining a spherical fully-connected layer with a hierarchical layer. This regularization is shown to improve the performance of widely used deep neural network architectures (ResNet and DenseNet) on publicly available datasets (CIFAR100, CUB200, Stanford dogs, Stanford cars, and Tiny-ImageNet).

## 1. Introduction

Applying *inductive biases* or prior knowledge to inference models is a popular strategy to improve their generalization performance (Battaglia et al., 2018). For example, a hierarchical structure can be found based on the similarity or shared characteristics between samples, and thus becomes a basic criterion to categorize particular objects. The *known* hierarchical structures provided by the datasets (e.g., birds taxonomy (Welinder et al., 2010) and WordNet hierarchy (Deng et al., 2009)) can help the network identify the similarity between the given samples.

In classification tasks, the last layer of neural networks maps embedding vectors to a discrete space (class). This mapping with a fully-connected layer has no mechanism forcing similar classes to be distributed close to each other in the embedding. Therefore, we may observe classes to be uniformly distributed after training, as this simplifies the categorization by the last fully-connected layer. This behavior is a consequence of seeing the label structure as ‘flat,’ i.e., it omits to consider the hierarchical relationships

between classes (Bilal et al., 2017).

To alleviate this problem, in this study, we force similar classes to be closer in the embedding by forcing their hyperplanes to follow a given hierarchy. One way to realize that is by making child nodes dependent on parent nodes and constraining their distance through a regularization term. However, the norm itself does not give relevant information on the closeness between hyperplanes (classifiers). Indeed, two classifiers are close if they classify two similar points in the same (super-)class. This means similar classifiers (hyperplanes) have to indicate a similar direction. Therefore, we have to focus on the *angle* between classifiers, which can be achieved through spherical constraints.

**Contributions.** In this paper, we propose a simple strategy to incorporate hierarchical information in deep neural network architectures with minimal changes to the training procedure, by *modifying only the last layer*. Given a hierarchical structure in the labels under the form of a tree, we explicitly force the individual classifiers to belong to a sphere, whose center is the classifier of their super-class, recursively until reaching the root (see Figure 2). We introduce the *spherical fully-connected layer* and the *hierarchically connected layer*, whose combination implements our proposed technique. We investigate the impact of Riemannian optimization instead of simple norm normalization. Finally, we empirically show that our proposed method makes embedding vectors distributed closely (clearly grouped) along similar classes with superior classification performances.

By its nature, our technique is quite versatile because it only affects the structure of last fully-connected layer of the neural network. Thus, it can be combined with many other strategies (like spherical CNN from Xie et al. (2017), or other deep neural network architectures).

**Related works.** Hierarchical structures are well-studied, and their properties can be effectively learned using manifold embedding. The design of the optimal embedding to learn the latent hierarchy is a complex task, and was extensively studied in the past decade. For example, Word2Vec (Mikolov et al., 2013b;a) and Poincaré embedding (Nickel & Kiela, 2017) showed a remarkable performance in hierarchical representation learning. (Du et al., 2018) forced the representation of sub-classes to “orbit” around the representation of their super-class to find similarity based embed-

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ding. Recently, using elliptical manifold embedding (Batmanghelich et al., 2016), hyperbolic manifolds (Nickel & Kiela, 2017; De Sa et al., 2018; Tifrea et al., 2018), and a combination of the two (Gu et al., 2019; Bachmann et al., 2019), shown that the latent structure of many data was non-Euclidean (Zhu et al., 2016; Bronstein et al., 2017; Skopek et al., 2019).

Mixing hierarchical information and structured prediction is not new, especially in text analysis (Koller & Sahami, 1997; McCallum et al., 1998; Weigend et al., 1999; Wang et al., 1999; Dumais & Chen, 2000). Partial order structure of the visual-semantic hierarchy is exploited using a simple order pair with max-margin loss function in (Vendrov et al., 2016). The results of previous studies indicate that exploiting hierarchical information during training gives better and more resilient classifiers, in particular when the number of classes is large (Cai & Hofmann, 2004). For a given hierarchy, it is possible to design structured models incorporating this information to improve the efficiency of the classifier. For instance, for support vector machines (SVMs), the techniques reported in (Cai & Hofmann, 2004; 2007; Gopal et al., 2012; Sela et al., 2011) use hierarchical regularization, forcing the classifier of a super-class to be close to the classifiers of its sub-classes. However, the intuition is very different in this case, because SVMs do not learn the embedding.

In this study, we consider that the hierarchy of the class labels is known. Moreover, we *do not* change prior layers of the deep neural network, and only work on the last layer that directly contribute to build hyperplanes for a classification purpose. Our work is thus orthogonal to those works on embedding learning, but not incompatible.

**Comparison with hyperbolic networks.** Hyperbolic network is a recent technique that showed impressive results for hierarchical representation learning. Poincaré networks (Nickel & Kiela, 2017) were originally designed to *learn* the latent hierarchy of data using *low-dimension* embedding. To alleviate their drawbacks due to a transductive property which cannot be used for unseen graph inference, hyperbolic neural networks equipped set aggregation operations have been proposed (Chami et al., 2019; Liu et al., 2019). These methods focus on learning embedding using a hyperbolic activation function for hierarchical representation. Our technique is orthogonal to these works: First, we assume that the hierarchical structure is not learned but already known. Second, our model focuses on generating individual hyperplanes of embedding vectors given by the network architecture. Therefore, our technique and hyperbolic networks *are not mutually exclusive*. Finally, even if this study focuses on spheres embedded in  $\mathbb{R}^d$ , it is straightforward to consider spheres embedded in hyperbolic spaces.

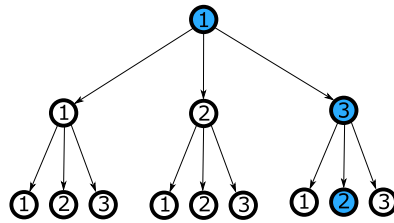


Figure 1. To reference the node at the bottom, we use the notation  $n_p$  with  $p = \{1, 3, 2\}$ . We use curly brackets  $\{ \}$  to write a path, and angle brackets  $\langle \cdot \rangle$  for the concatenation of paths.

## 2. Hierarchical Regularization

### 2.1. Definition and Notations

We assume we have samples with hierarchically ordered classes. For instance, apple, banana, and orange are classes that may belong to the super-class “fruits.” This represents hierarchical relationships with trees, as depicted in Figure 1.

We identify nodes in the graph through their path. To represent the leaf (highlighted in blue in Figure 1), we use the notation  $n_{\{1,3,2\}}$ . This means it is the second child of the super-class  $n_{\{1,3\}}$ , and recursively, until we reach the root.

More formally, we identify nodes as  $n_p$ , where  $p$  is the path to the node. A path uniquely defines a node where only one possible path exists. Using the concatenation, between the path  $p$  and its child  $i$ , a new path  $\tilde{p}$  can be defined as follows,

$$\tilde{p} = \langle p, i \rangle \quad (1)$$

We denote  $\mathcal{P}$  the set of all paths in the tree starting from the root, with cardinality  $|\mathcal{P}|$ . Notice that  $|\mathcal{P}|$  is also the number of nodes in the tree (i.e., number of classes and super-classes). We distinguish the set  $\mathcal{P}$  from the set  $\mathcal{L}$ , the set of paths associated to nodes whose label appears in the dataset. Although  $\mathcal{L}$  may equal to  $\mathcal{P}$ , this is not the case in our experiments. We show an example in Appendix A.

### 2.2. Similarity Between Objects and Their Representation

Let  $X$  be the network input (e.g. an image), and  $\phi_\theta(X)$  be its representation, i.e., the features of  $X$  extracted by a deep neural network parameterized by  $\theta$ . We start with the following observation:

*Given a representation, super-class hyperplane should be similar to hyperplanes for their sub-classes.*

This assumption implies the following direct consequence.

*All objects whose labels belong to the same super-class have a similar representation.*

That is a natural property that we may expect from a good representation. For instance, two dogs from different breeds should share more common features than that of a dog shares with an apple. Therefore, the parameter of the classifiers that identify dog’s breed should also be similar. Their difference lies in the parameters associated to some specific features that differentiate breeds of dogs.

Although this is not necessarily satisfied with *arbitrary* hierarchical classification, we observe this in many existing datasets. For instance, Caltech-UCSD Birds 200 and Stanford dogs are datasets that classify, respectively, birds and dogs in term of their breeds. A possible example where this assumption may not be satisfied is a dataset whose super-classes are “labels whose first letter is «.»”

### 2.3. Hierarchical Regularization

Starting from a simple observation in the previous section, we propose a regularization method that forces the network to have similar representation for classes along a path  $p$ , which implies having similar representation between similar objects. More formally, if we have an optimal classifier  $w_p$  for the super-class  $p$  and a classifier  $w_{\langle p,i \rangle}$  for the class  $\langle p, i \rangle$ , we expect that

$$\|w_p - w_{\langle p,i \rangle}\| \text{ is small.} \quad (2)$$

If this is satisfied, hyperplanes for objects in the same super-class are also similar because

$$\begin{aligned} \|w_{\langle p,i \rangle} - w_{\langle p,j \rangle}\| &= \|(w_{\langle p,i \rangle} - w_p) - (w_{\langle p,j \rangle} - w_p)| \\ &\leq \underbrace{\|w_p - w_{\langle p,i \rangle}\|}_{\text{small}} + \underbrace{\|w_p - w_{\langle p,j \rangle}\|}_{\text{small}}. \end{aligned} \quad (3)$$

However, the optimal hyperplane (classifier) for an arbitrary representation  $\phi_\theta(X)$  may not satisfy (2). The naive and direct way to ensure (2) is through *hierarchical regularization*, which forces hyperplanes (classifiers) in the same path to be close to each other.

### 2.4. Hierarchical Layer and Hierarchically Connected Layer

In the previous section, we described the hierarchical regularization method given a hierarchical structure in the classes. In this section, we show how to conveniently parametrize (2). We first express the hyperplane (classifier) as a sum of vectors  $\delta$  defined recursively as follows:

$$w_{\langle p,i \rangle} = w_p + \delta_{\langle p,i \rangle}, \quad \delta_{\{\}} = \mathbf{0}, \quad (4)$$

where  $\{\}$  is the root. It is possible to consider  $\delta_{\{\}} \neq \mathbf{0}$ , which shifts separating hyperplanes. We do not consider this case in this paper. Given (4), we have that  $\|\delta_{\langle p,i \rangle}\|$  is

small in (2). Finally, it suffices to penalize the norm of  $\delta_{\langle p,i \rangle}$  during the optimization. Notice that, by construction, the number of  $\delta$ ’s is equal to the number of nodes in the hierarchical tree.

Next, consider the output of CNNs for classification,

$$\phi_\theta(\cdot)^T W, \quad (5)$$

where  $\theta$  denotes the parameters of the hidden layers,  $W = [w_1, \dots, w_{|\mathcal{L}|}]$  denotes the last fully-connected layer, and  $w_i$  denotes the classifier for the class  $i$ . For simplicity, we omit potential additional nonlinear functions, such as a softmax, on top of the prediction.

We have parametrized  $w_i$  following the recursive formula in (4). To define the matrix formulation of (4), we first introduce the *Hierarchical layer*  $\mathbf{H}$  which plays an important role. This hierarchical layer can be identified to the adjacency matrix of the hierarchical graph.

**Definition 1. (Hierarchical layer).** Consider ordering over the sets  $\mathcal{P}$  and  $\mathcal{L}$ , i.e., for  $i = 1, \dots, |\mathcal{P}|$  and  $j = 1, \dots, |\mathcal{L}|$ ,

$$\mathcal{P} = \{p_1, \dots, p_i, \dots, p_{|\mathcal{P}|}\} \text{ and } \mathcal{L} = \{p_1, \dots, p_j, \dots, p_{|\mathcal{L}|}\}.$$

In other words, we associate to all nodes an index. Then, the hierarchical layer  $\mathbf{H}$  is defined as

$$\mathbf{H} \in \{0, 1\}^{|\mathcal{P}| \times |\mathcal{L}|}, \quad \mathbf{H}_{i,j} = 1 \text{ if } n_{p_i} \preceq n_{p_j}, \quad 0 \text{ otherwise.} \quad (6)$$

where  $n_{p_i} \preceq n_{p_j}$  means  $n_{p_j}$  is a parent of  $n_{p_i}$ .

We illustrate an example of  $\mathbf{H}$  in Appendix A. The next proposition shows that (5) can be written using a simple matrix-matrix multiplication, involving the hierarchical layer.

**Proposition 1.** Consider a representation  $\phi_\theta(\cdot)$ , where  $\phi_\theta(\cdot) \in \mathbb{R}^d$ . Let  $W$  be the matrix of hyperplanes

$$W = [w_{p_1}, \dots, w_{p_{|\mathcal{L}|}}], \quad p_i \in \mathcal{L}, \quad (7)$$

where the hyperplanes are parametrized as (4). Let  $\Delta$  be defined as

$$\Delta \in \mathbb{R}^{d \times |\mathcal{P}|}, \quad \Delta = [\delta_{p_1}, \dots, \delta_{p_{|\mathcal{P}|}}], \quad (8)$$

where  $\mathcal{P}$  and  $\mathcal{L}$  are defined in Section 2.1. Consider the hierarchical layer defined in Definition 1. Then, the matrix of hyperplanes  $W$  can be expressed as

$$W = \Delta \mathbf{H}. \quad (9)$$

We can see  $W = \Delta \mathbf{H}$  as a combination of an augmented fully-connected layer, combined with the hierarchical layer that selects the corresponding columns of  $\Delta$ , hence the term *hierarchically connected layer*. The  $\ell_2$  regularization of the

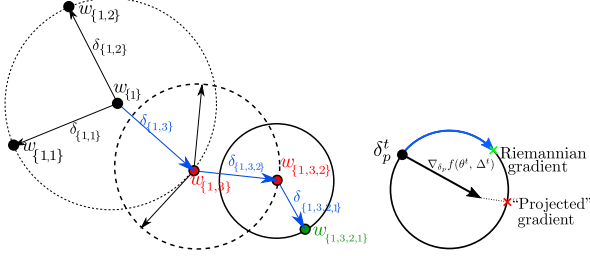


Figure 2. **(Left)** Example of hyperplanes  $w_p$ , formed through the sum of  $\delta_p$ . The hyperplane  $w_{\{1,3,2,1\}}$  associated to the class  $n_{\{1,3,2,1\}}$  is in green, the construction with the  $\delta$ 's in blue, and all intermediate  $w$  in red. **(Right)** Riemannian versus “projected” gradient descent. Riemannian optimization follows approximately geodesics, while projected gradient steps can jump very far from  $\delta_p^t$ .

$\delta$  can be conducted by the parameter *weight decay*, which is widely used in training of neural networks. The hierarchical layer  $\mathbf{H}$  is fixed, while  $\Delta$  is learnable. This does not affect the complexity of the back-propagation significantly, as  $\Delta\mathbf{H}$  is a simple linear form.

The size of the last layer slightly increases, from  $|\mathcal{L}| \times d$  to  $|\mathcal{P}| \times d$ , where  $d$  is the dimension of the representation  $\phi_\theta(\cdot)$ . For instance, in the case of Tiny-ImageNet, the number of parameters of the last layer only increases by roughly 36%; nevertheless, the increased number of parameters of the last layer is still usually negligible in comparison with the total number of parameters for classical network architectures.

### 3. Hierarchical Spheres

The *hierarchical* ( $\ell_2$ ) regularization introduced in the previous section induces separated hyperplanes along a path to be close to each other. However, this approach has a significant drawback.

We rewind (2), which models the similarity of two hyperplanes  $w_p$  and  $w_{\langle p, i \rangle}$ . The similarity between hyperplanes (individual hyperplanes) should indicate that they point roughly the same direction, i.e.,

$$\left\| \frac{w_p}{\|w_p\|} - \frac{w_{\langle p, i \rangle}}{\|w_{\langle p, i \rangle}\|} \right\| \text{ is small.} \quad (10)$$

However, this property is *not* necessarily captured by (2). For instance, assume that  $w_p = -w_{\langle p, i \rangle}$ , i.e., the hyperplanes point in two opposite directions (and thus completely different). Then, (2) can be arbitrarily small in the function of  $\|w_p\|$  but not in (10):

$$\|w_p - w_{\langle p, i \rangle}\| = 2\|w_p\| \quad ; \quad \left\| \frac{w_p}{\|w_p\|} - \frac{w_{\langle p, i \rangle}}{\|w_{\langle p, i \rangle}\|} \right\| = 2. \quad (11)$$

This can be avoided, for example, by deploying the regularization parameter (or weight decay) independently for

each  $\|\delta_p\|$ . However, it is costly in terms of hyper-parameter estimation.

In order to enforce the closeness of embedding vectors whose paths are similar, we penalize large norms of  $\delta$ . We also want to bound it away from zero to avoid the problem of hyperplanes that point in different direction may have a small norm. This naturally leads to a spherical constraint. Indeed, we transform the  $\ell_2$  regularization over  $\delta_p$  by fixing its norm in advance, i.e.,

$$\|\delta_p\| = R_p > 0. \quad (12)$$

In other words, we define  $\delta_p$  on a sphere of radius  $R_p$ . The fully-connected layer  $\Delta$  is then constrained on spheres, hence it is named *spherical fully-connected layer*.

Hence, we have  $w_{\langle p, i \rangle}$  constrained on a sphere centered at  $w_p$ . This constraint prevents the direction of  $w_{\langle p, i \rangle}$  from being too different from that of  $w_p$ , while bounding the distance away from zero. This does not add hyperparameters: instead of weight decay, we have the radius  $R_p$  of the sphere.

#### 3.1. Radius Decay w.r.t. Path Length

We allow the radius of the spheres,  $R_p$ , to be defined as a function of the path. In this study, we use a simple strategy called *radius decay*, where  $R_p$  decreases w.r.t. the path length:

$$R_p = R_0 \gamma^{|p|}, \quad (13)$$

where  $R_0$  is the initial radius,  $\gamma$  is the radius decay parameter, and  $|p|$  is the length of the path. The optimal radius decay can be easily found using cross-validation. The radius decay is applied prior to learning (as opposed to weight-decay); then, the radius remains fixed during the optimization. As opposed to weight-decay, whose weight are multiplied by some constant smaller than one after each iteration, the radius decay here depends only on the path length, and the radius remains fixed during the optimization process.

The simplest way to apply the radius decay is by using the following predefined diagonal matrix  $\mathbf{D}$ ,

$$\mathbf{D}_{i, i} = R_0 \gamma^{|p_i|}, \quad p_i \in \mathcal{P}, \quad 0 \text{ otherwise,} \quad (14)$$

where  $p_i$  follows the ordering from Definition 1. Finally, the last layer of the neural network reads,

$$\underbrace{\phi_\theta(\cdot)}_{\text{Network}} \underbrace{\Delta \mathbf{D} \mathbf{H}}_{\text{Last layer}}. \quad (15)$$

The only learnable parameter in the last layer is  $\Delta$ .



### 3.2. Optimization

There are several ways to optimize the network in the presence of the *spherical fully-connected layer*: by introducing the constraint in the model, “naively” by performing normalization after each step, or by using Riemannian optimization algorithms. For simplicity, we consider the minimization problem,

$$\min_{\theta, \Delta} f(\theta, \Delta), \quad (16)$$

where  $\theta$  are the parameters of the hidden layers,  $\Delta$  the spherical fully-connected layer from (8), and  $f$  the empirical expectation of the loss of the neural network. For clarity, we use noiseless gradients, but all results also apply to stochastic ones. The superscript  $\cdot^t$  denotes the  $t$ -th iteration.

**Integration of the constraint in the model.** We present the simplest way to force the column of  $\Delta$  to lie on a sphere, as this does not require a dedicated optimization algorithm. It is sufficient to normalize the column of  $\Delta$  by their norm in the model. By introducing a dummy variable  $\tilde{\Delta}$ , which is the normalized version of  $\Delta$ , the last layer of the neural network (15) reads

$$\tilde{\Delta} = [\dots, \frac{\delta_p}{\|\delta_p\|}, \dots], \quad \phi_{\theta}(\cdot) \tilde{\Delta} \mathbf{D} \mathbf{H}. \quad (17)$$

Then, any standard optimization algorithm can be used for the learning phase. Technically,  $\Delta$  is *not* constrained on a sphere, but the model will act as if  $\Delta$  follows such constraint.

**Optimization over spheres—Riemannian (stochastic) gradient descent.** The most direct way to optimize over a sphere is to normalize the columns of  $\Delta$  by their norm after each iteration. However, this method has no convergence guarantee, and requires a modification in the optimization algorithm. Instead, we perform Riemannian gradient descent which we explain only briefly in this manuscript. We provide the derivation of Riemannian gradient for spheres in Appendix B.

Riemannian gradient descent involves two steps: first, a projection to the tangent space, and then, a retraction to the manifold. The projection step computes the gradient of the function *on the manifold* (as opposed to the ambient space  $\mathbb{R}^d$ ), such that its gradient is *tangent* to the sphere. Then, the retraction simply maps the new iterate to the sphere. With this two-step procedure, all directions pointing *outside* the manifold, (i.e., orthogonal to the manifold, thus irrelevant) are discarded by the projection. These two steps are summarized below,

$$s^t = (\delta_p^t)^T \nabla_{\delta_p} f(\theta^t, \Delta^t) \cdot \delta_p^t - \nabla_{\delta_p} f(\theta^t, \Delta^t), \quad (18)$$

$$\delta_p^{t+1} = \frac{\delta_p^t + h^t s^t}{\|\delta_p^t + h^t s^t\|}, \quad (19)$$

where  $s^t$  is the projection of the descent direction to the tangent space, and  $\delta_p^{t+1}$  is the retraction of the gradient descent step with stepsize  $h$ . In our experiments, we used the Geopt optimizer (Kochurov et al., 2020), which implements Riemannian gradient descent on spheres.

## 4. Experiments

We experimented the proposed method using five publicly available datasets, namely CIFAR100 (Krizhevsky, 2009), Caltech-UCSD Birds 200 (CUB200) (Welinder et al., 2010), Stanford-Cars (Cars) (Krause et al., 2013), Stanford-dogs (Dogs) (Khosla et al., 2011), and Tiny-ImageNet (Tiny-ImNet) (Deng et al., 2009). CUB200, Cars, and Dogs datasets are used for fine-grained categorization (recognizing bird, dog breeds, or car models), while CIFAR100 and Tiny-ImNet datasets are used for the classification of objects and animals. Unlike the datasets for object classification, the fine-grained categorization datasets show low inter-class variances. See Appendix C.2 and C.3 for more details about the dataset and their hierarchy, respectively.

### 4.1. Deep Neural Network Models and Training setting

We used the deep neural networks (*ResNet* (He et al., 2016) and *DenseNet* (Huang et al., 2017)). The input size of the datasets CUB200, Cars, Dogs, and Tiny-ImNet is  $224 \times 224$  (for Tiny-ImNet, resized from  $64 \times 64$ ), and  $32 \times 32$  pixels for CIFAR100. Since the input-size of CIFAR100 does not fit to the original ResNet and DenseNet, we used a smaller kernel size (3 instead of 7) at the first convolutional layer and a smaller stride (1 instead of 2) at the first block.

**Remark: we do not use pretrained models.** All networks used in the experiments are trained from scratch, i.e., we did not employ fine-tuning or transfer learning strategies using the pretrained models. This is because most publicly available pretrained models used ImageNet for training while images in CUB200, Dogs and Tiny-ImNet overlap with the ones from ImageNet.

We used the stochastic gradient descent (SGD) over 300 epochs, with a mini-batch of 64 and a momentum parameter of 0.9 for training. The learning rate schedule is the same for all experiments, starting at 0.1, then decaying by a factor of 10 after 150, then 225 epochs. All tests are conducted using NVIDIA Tesla V100 GPU with the same random seed. Settings in more detail are provided in the supplementary material. We emphasize that we used the same parameters and learning rate schedule for *all scenarios*. Those parameters and schedule were optimized for SGD on plain networks, but are probably sub-optimal for our proposed methods.

Table 1. Test accuracy (%) for fine-grained classification. Radius decay is fixed at 0.5.

Dataset	Architecture	Baseline		Proposed parametrization		
		Plain	Multitask	Hierarchy	+Manifold	+Riemann
CUB200	ResNet-18	54.88	53.99	58.28	60.42	<b>60.98</b>
	ResNet-50	54.09	52.17	57.59	59.00	<b>60.01</b>
	DenseNet-121	50.55	56.61	61.10	60.22	<b>61.98</b>
	DenseNet-161	50.91	60.67	60.67	62.73	<b>63.55</b>
Cars	ResNet-18	79.83	82.85	<b>84.96</b>	84.74	84.16
	ResNet-50	82.86	82.86	83.34	84.51	<b>84.65</b>
	DenseNet-121	79.78	85.39	85.97	<b>86.00</b>	85.54
	DenseNet-161	79.85	85.79	86.23	<b>86.90</b>	85.76
Dogs	ResNet-18	59.17	59.88	60.30	<b>61.83</b>	61.36
	ResNet-50	57.44	58.97	59.31	59.81	<b>63.70</b>
	DenseNet-121	56.00	64.39	62.19	64.95	<b>65.89</b>
	DenseNet-161	55.49	64.23	65.28	65.68	<b>65.90</b>

Table 2. Test accuracy (%) for object classification. Radius decay is fixed at 0.5 and 0.9 for CIFAR100 and Tiny-Imnet, respectively.

Dataset	Architecture	Baseline		Proposed parametrization		
		Plain	Multitask	Hierarchy	+Manifold	+Riemann
CIFAR100	ResNet-18	69.47	69.37	70.89	70.06	<b>71.89</b>
	ResNet-50	71.04	71.74	73.75	73.76	<b>73.97</b>
	DenseNet-121	74.50	75.62	76.38	<b>76.52</b>	76.28
	DenseNet-161	75.30	76.57	77.01	<b>77.01</b>	76.64
Tiny-ImNet	ResNet-18	64.70	64.81	64.33	64.74	<b>65.13</b>
	ResNet-50	66.43	66.39	66.52	<b>66.67</b>	65.69
	DenseNet-121	64.27	67.15	67.19	<b>67.86</b>	67.45
	DenseNet-161	67.22	67.62	67.63	<b>68.95</b>	67.82

 Table 3. Comparison with hyperbolic networks (Khurlov et al., 2020): test accuracy (%) for fine-grained (top) or objects (bottom) classification, using ResNet-18. The number in parenthesis is the STD over 6 runs with different random seeds.  $lr$  denotes the initial learning rate.

Dataset	Hyperbolic ( $lr$ : 0.01)	Hyperbolic ( $lr$ : 0.001)	Hyperbolic ( $lr$ : 0.0001)	Ours (+Riemann)
CUB200	7.49 ( $\pm 0.68$ )	40.14 ( $\pm 0.49$ )	26.93 ( $\pm 0.50$ )	<b>61.62</b> ( $\pm 0.35$ )
Cars	15.79 ( $\pm 16.54$ )	62.41 ( $\pm 0.86$ )	42.40 ( $\pm 1.23$ )	<b>83.41</b> ( $\pm 0.54$ )
Dogs	18.70 ( $\pm 12.95$ )	48.85 ( $\pm 0.59$ )	40.19 ( $\pm 0.23$ )	<b>61.35</b> ( $\pm 0.37$ )
CIFAR-10	42.30 ( $\pm 7.66$ )	56.37 ( $\pm 10.45$ )	59.67 ( $\pm 0.37$ )	<b>71.82</b> ( $\pm 0.18$ )
TinyImNet	14.53 ( $\pm 11.17$ )	48.83 ( $\pm 13.16$ )	53.17 ( $\pm 0.29$ )	<b>64.93</b> ( $\pm 0.18$ )

## 4.2. Results

Tables 1 and 2 show a comparison of the results obtained with several baseline methods and our methods. The first method, “Plain”, is a plain network for subclass classification without hierarchical information. The second one, “Multitask” is simply the plain network with multitask (subclass and super-class classification) setting using the hierarchical information. The third one, “Hierarchy”, uses our parametrization  $W = \Delta \mathbf{H}$  with the hierarchical layer  $\mathbf{H}$ , but the columns of  $\Delta$  are not constrained on spheres. Then, “+Manifold” means that  $\Delta$  is restricted on a sphere using the normalization technique from Section 3.2 (Integration of the constraint in the model). Finally, “+Riemann” means

we used Riemannian optimization from Section 3.2 (Optimization over spheres). We show the experimental results on fine-grained classification (Table 1) and general object classification (Table 2).

Note that the *multitask* strategy in our experiment (and contrary to our regularization method) does require an additional hyper-parameter that combines the two losses, because we train classifiers for super-classes and sub-classes simultaneously.

**Fine-grained categorization.** As shown in Table 1, our proposed parameterization significantly improves the test accuracy over the baseline networks (ResNet-18/50 and

DenseNet-121/160). Even the simple hierarchical setting which uses the hierarchical layer only (without spheres) shows superior performance compared to the baseline networks. Integrating the manifolds with Riemannian SGD further improves the generalization performance.

Surprisingly, the plain network with deeper layers shows degraded performance. This can be attributed to overfitting which does not occur with our regularization method, where larger networks show better performance, indicating the high efficiency of our approach.

**Object classification.** We show test accuracy (%) of our proposed methods with different network models using CIFAR-100 and Tiny-ImNet, in Table 2. As shown in the table, our proposed method has better classification accuracy than that of the baseline methods. Compared to the fine-grained classification datasets, the general object classification datasets have less similar classes on the same super-class. In these datasets, our method achieved relatively small gains. A higher inter-class variance may explain the lower improvement compared to fine-grained categorization.

For Tiny-ImNet, ResNet-18 (11.28M param.) with our parametrization achieves better classification performance than plain ResNet-50 (23.91M param.). The same applies to DenseNet-121 and DenseNet-161. These results indicate that our regularization method, *which does not introduce new parameters in the embedding layer*, can achieve a classification performance similar than more complex models.

**Comparison with hyperbolic networks.** Hyperbolic networks using Poincaré ball based Multidimensional Logistic Regression (MLR) (Khrulkov et al., 2020; Shimizu et al., 2021) can be used for the classification task. Khrulkov et al. (2020) showed improved performance on shallow networks with four convolutional layers for image classification with few-shot learning, but not on deep networks, e.g., ResNet12. Shimizu et al. (2021) showed improved performance on subtree classification (binary classification for each node) and for language translation tasks when using low dimensional embeddings ( $\leq 10$  and  $\leq 64$ , respectively).

Table 3 compares our method with the hyperbolic networks for object classification. We report the averaged test accuracy of six runs of hyperbolic model (Poincaré ball based MLR) where MLR layers are added to ResNet-18 (512 dimensional embedding) based on the codes from (Khrulkov et al., 2020). We compare those results with our method (Hierarchy+Manifold+Riemann). For the experiments, we followed training settings described in Section 4.1 except for the initial learning rate ( $lr$ ). Without an extensive hyperparameter search, the method easily diverges, as it is very sensitive to the radius and initial learning rate, as described in (Khrulkov et al., 2020). This Hyperbolic method using deeper networks on higher dimensional embedding space

showed unstable and degraded performances for visual object classification compared to our proposed method.

### 4.3. Riemannian vs. Projected SGD

Overall, Riemannian SGD showed slightly superior performance compared to projected SGD for fine-grained datasets, although, in most cases, the performance was similar. For instance, with the *Dogs* dataset on ResNet-50, Riemannian SGD shows a performance 4% higher than the projected SGD. For object classification, Riemannian SGD improves the classification performance a bit less compared to that the projected SGD. For the different radius decay parameters (0.5 in Table 1 and 0.9 in Table 2), the optimized learning rate (e.g. with a large value) of Riemannian SGD may improve the performance further.

### 4.4. Ablation Study

In this section, we conduct an ablation study with different perspectives to answer following questions: 1) *Can learnable sphere radius be more effective than fixed radius decay*, and 2) *is hierarchical modeling really effective?*

Table 4. Test accuracy (%) with a **learnable radius**. Clearly, using learnable parameter degrades considerably the performance compared to using the predefined radius decay (shown in parentheses, selected from Table 1). ResNet-18.

Dataset	Proposed parametrization		
	Hierarchy	+Manifold	+Riemann
CUB200	53.40 (58.28)	58.35 (60.42)	58.24 (60.98)
Cars	81.51 (84.96)	82.54 (84.74)	82.40 (84.16)

Table 5. Test accuracy (%) with a **random hierarchy tree**. Radius decay is fixed at 0.5. Clearly, using a random hierarchy degrades considerably the performance (shown in parentheses, selected from Table 1 which are the results with the original hierarchical tree). This validates the importance of the proper hierarchy information. ResNet-18.

Dataset	Baseline	Proposed parametrization		
	Multitask	Hierarchy	+Manifold	+Riemann
CUB200	47.55 (53.99)	50.28 (58.28)	56.96 (60.42)	56.43 (60.98)
Cars	79.98 (82.85)	81.07 (84.96)	82.02 (84.74)	81.84 (84.16)

Table 6. Test accuracy (%) for **super-class classification**. Radius decay is fixed at 0.5. For the super-class classification, without any modification of the proposed layers, we trained the model on the dataset, then calculated classification accuracy using the  $\delta$ 's corresponding to the parent classes. ResNet-18.

Dataset	Baseline	Proposed parametrization		
	Multitask	Hierarchy	+Manifold	+Riemann
CUB200	53.68	58.87	61.17	<b>62.22</b>
Cars	86.88	87.91	<b>91.23</b>	90.97

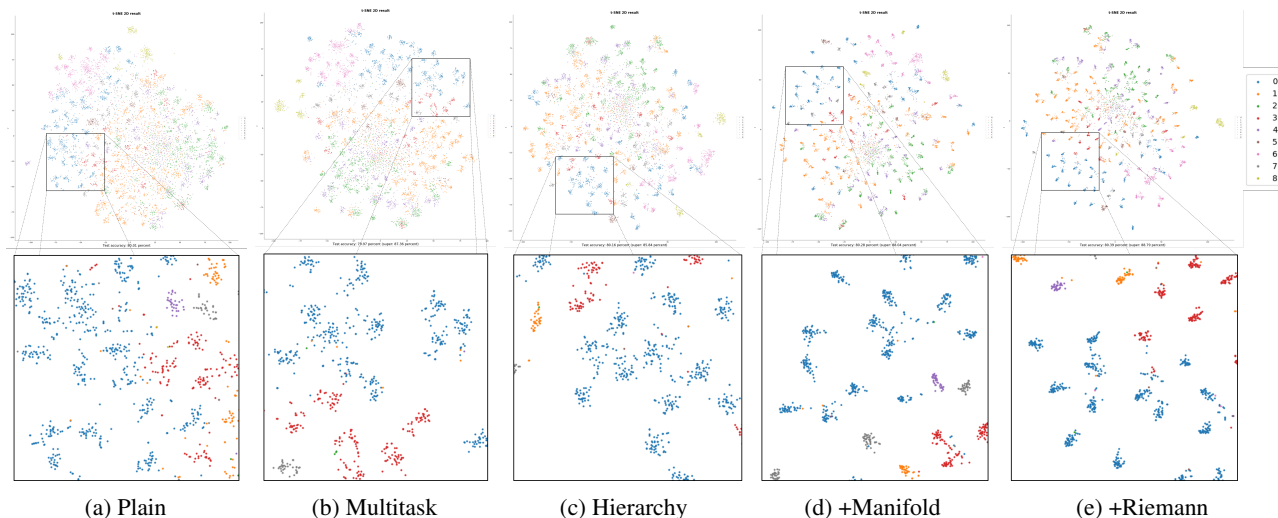


Figure 3. Visualization of a high dimensional embedding vector using t-SNE on 2D plane (using ResNet-18 and Cars dataset). We show zoom-in figure highlighted with black solid rectangle by cropping sample distribution having similar super-classes for clarity. (a) Plain, (b) Multitask, and proposed parameterization ((c) Hierarchy, (d) +Manifold, and (e) +Riemann). In overall, our proposed methods ((c), (d), (e)) show clearer separation among similar super-classes with smaller deviation. All figures are drawn using embedding vectors shown the similar classification accuracy (approximately 80 %, maximum performance of the baseline) for fairness.

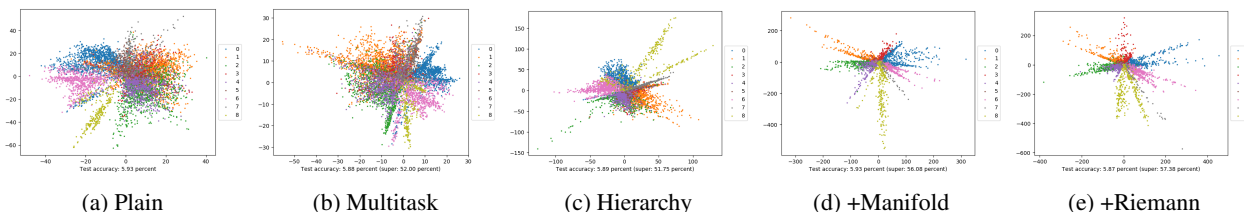


Figure 4. Visualization of 2-dimensional embedding vector (using ResNet-18 and Cars dataset). (a) Plain, (b) Multitask, and proposed parameterization ((c) Hierarchy, (d) +Manifold, and (e) +Riemann). Our proposed methods draw that samples with 196 sub-classes are grouped sharply along with 9 super-classes compared to the baseline methods, i.e., the distribution of points becomes more and more concentrated and separable. We showed the distribution from low accuracy (approx. 6 % accuracy). Two-dimensional vectors seem too small to classify images of 196 classes which is highly non-linearly distributed different from MNIST dataset with ten classes and gray level images shown in (Liu et al., 2016).

**Learnable sphere radius.** Instead of the predefined simple radius decay equation in (13), represented by the diagonal matrix  $\mathbf{D}$  in (14), we replace it with a learnable diagonal matrix of parameters which is trainable using backpropagation. As shown in Table 4, this learnable radius is not effective in terms of a classification performance, compared to the one of the predefined depth-wise radius decay.

**Importance of hierarchy.** To validate the hierarchical (manually annotated) label structure used in the experiments and the proposed hierarchical sphere modeling further, we observe their performances from three different perspectives, *Randomized hierarchy*, *Super-class categorization*, and *Embedding distribution* as follows.

*Randomized hierarchical structure* (Table 5). We examine hierarchical modeling using random hierarchical labels to

validate the importance of the given hierarchy labels from the dataset. One can propose to use labels found in an unsupervised way. However, popular (and simple) unsupervised clustering, or grouping, method such as *k-mean*, provides randomly assigned super-class labels. Hence, we examine simply a random super-class assignment. As shown in Table 5, the methods with a randomly generated hierarchy shows a degraded performance compared to that with a given hierarchical information. This validates the effectiveness of the hierarchy structure we used in the above experiments.

*Super-class categorization accuracy* (Table 6). As shown in Table 6, our proposed methods (Hierarchy, +Manifold, and +Riemann) outperformed a baseline hierarchical (multitask) method in terms of test accuracy performance. Note that, in the multitask classification, a loss function for classi-



fication using super-classes is used additionally. This result validates that our proposed methods work in a hierarchical way. Modeling on spheres (+Manifold and +Riemann) further improves hierarchical inference.

*Visualization of embedding vectors (Figures 3 and 4).* We show a distribution of embedding vectors to observe how our proposed modeling draws the input samples in groupwise setting. We visualize both the original (high-dimensional) embedding used in above experiments and small dimensional embedding vectors using Cars dataset (the number of superclasses is small enough to show their distribution clearly).

We use a popular visualization technique, t-Distributed Stochastic Neighbor Embeddings (t-SNE) (van der Maaten & Hinton, 2008), to visualize the embedding vector ( $\mathbb{R}^{512}$ ) in a two-dimensional space. As shown in Figure 3, embedding vectors of our proposed methods (see Figure 3c, 3d, and 3e) are clearly grouped within small distance for each sub-class and their super-classes (the same color indicates the same super-class) compared to that of the baseline methods (see Figure 3a and 3b).

Since t-SNE returns stochastic results dependent on hyperparameters such *perplexity* values but independent to the networks, we visualize two-dimensional vector ( $\mathbb{R}^2$ ) directly learned by the networks following (Liu et al., 2016). To obtain this embedding vector, we added an additional (dimensionality reduction) layer (i.e. a mapping function  $\mathbb{R}^{512} \mapsto \mathbb{R}^2$ ) prior to the last FC layer of ResNet-18. As shown in Figure 4, embedding vectors of our proposed methods are distributed more closely (clustered) with regard to their super-classes (Figure 4c, 4d, and 4e).

## 5. Conclusion and Future Work

We presented a simple regularization method for neural networks using a given hierarchical structure of the classes. We reformulated the fully connected layer which is the last layer of the neural network using the *hierarchical layer*. By applying spherical constraints to this layer further, we formulated a *spherical fully-connected layer*. The reformulation using the hierarchical layer  $\Delta\mathbf{H}$  and the spherical constraint had a considerable impact on the generalization accuracy of the network. Finally, we compared several optimization strategies for the spherical layer. The Riemannian optimization showed significant improvement and sometimes similar to its projected counterpart.

In the future, it would be interesting to use our proposed regularization method on other architectures (e.g. Inception and SqueezeNet), for embedding (e.g. Poincaré), and other applications (e.g. Natural Language Processing). Moreover, in this paper, we used a given hierarchy mostly based on taxonomy designed by experts. This hierarchical structure,

which is convenient for humans, may not be most convenient for classification algorithms. Alternatively, a self-supervised algorithm that learns the hierarchy and classifier simultaneously may be effective because we do not need to access a given hierarchy and lead to better results (because the structure will be more adapted to the classification task).

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## References

- Absil, P.-A., Mahony, R., and Sepulchre, R. *Optimization Algorithms on Matrix Manifolds*. Princeton University Press, Princeton, NJ, USA, 2007. ISBN 0691132984, 9780691132983.
- Bachmann, G., Bécigneul, G., and Ganea, O.-E. Constant curvature graph convolutional networks. *arXiv preprint arXiv:1911.05076*, 2019.
- Batmanghelich, K., Saeedi, A., Narasimhan, K., and Gershman, S. Nonparametric spherical topic modeling with word embeddings. In *Proceedings of the conference. Association for Computational Linguistics. Meeting*, volume 2016, pp. 537. NIH Public Access, 2016.
- Battaglia, P., Hamrick, J. B. C., Bapst, V., Sanchez, A., Zambaldi, V., Malinowski, M., Tacchetti, A., Raposo, D., Santoro, A., Faulkner, R., Gulcehre, C., Song, F., Ballard, A., Gilmer, J., Dahl, G. E., Vaswani, A., Allen, K., Nash, C., Langston, V. J., Dyer, C., Heess, N., Wierstra, D., Kohli, P., Botvinick, M., Vinyals, O., Li, Y., and Pascanu, R. Relational inductive biases, deep learning, and graph networks. *arXiv*, 2018.
- Bécigneul, G. and Ganea, O.-E. Riemannian adaptive optimization methods. *arXiv preprint arXiv:1810.00760*, 2018.
- Bilal, A., Jourabloo, A., Ye, M., Liu, X., and Ren, L. Do convolutional neural networks learn class hierarchy? *IEEE transactions on visualization and computer graphics*, 24(1):152–162, 2017.
- Bonnabel, S. Stochastic gradient descent on riemannian manifolds. *IEEE Transactions on Automatic Control*, 58(9):2217–2229, Sep. 2013.
- Boumal, N. An introduction to optimization on smooth manifolds. Available online, May 2020. URL <http://www.nicolasboumal.net/book>.
- Bronstein, M. M., Bruna, J., LeCun, Y., Szlam, A., and Vandergheynst, P. Geometric deep learning: going beyond euclidean data. *IEEE Signal Processing Magazine*, 34(4): 18–42, 2017.
- Cai, L. and Hofmann, T. Hierarchical document categorization with support vector machines. In *Proceedings of the thirteenth ACM international conference on Information and knowledge management*, pp. 78–87, 2004.
- Cai, L. and Hofmann, T. Exploiting known taxonomies in learning overlapping concepts. In *IJCAI*, volume 7, pp. 708–713, 2007.
- Chami, I., Ying, Z., Ré, C., and Leskovec, J. Hyperbolic graph convolutional neural networks. In *Advances in Neural Information Processing Systems 32*, pp. 4868–4879, 2019.
- De Sa, C., Gu, A., Ré, C., and Sala, F. Representation tradeoffs for hyperbolic embeddings. *Proceedings of machine learning research*, 80:4460, 2018.
- Deng, J., Dong, W., Socher, R., Li, L.-J., Li, K., and Fei-Fei, L. ImageNet: A Large-Scale Hierarchical Image Database. In *CVPR09*, 2009.
- Du, L., Lu, Z., Wang, Y., Song, G., Wang, Y., and Chen, W. Galaxy network embedding: A hierarchical community structure preserving approach. In *IJCAI*, pp. 2079–2085, 2018.
- Dumais, S. and Chen, H. Hierarchical classification of web content. In *Proceedings of the 23rd annual international ACM SIGIR conference on Research and development in information retrieval*, pp. 256–263, 2000.
- Gopal, S., Yang, Y., and Niculescu-Mizil, A. Regularization framework for large scale hierarchical classification. *Proceedings of European Conference on Machine Learning*, 2012.
- Gu, A., Sala, F., Gunel, B., and Ré, C. Learning mixed-curvature representations in product spaces. In *International Conference on Learning Representations*, 2019.
- He, K., Zhang, X., Ren, S., and Sun, J. Deep residual learning for image recognition. In *2016 IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2016, Las Vegas, NV, USA, June 27-30, 2016*, pp. 770–778, 2016.
- Huang, G., Liu, Z., van der Maaten, L., and Weinberger, K. Q. Densely connected convolutional networks. In *CVPR*, pp. 2261–2269. IEEE Computer Society, 2017.
- Khosla, A., Jayadevaprakash, N., Yao, B., and Fei-Fei, L. Novel dataset for fine-grained image categorization. In *First Workshop on Fine-Grained Visual Categorization, IEEE Conference on Computer Vision and Pattern Recognition*, Colorado Springs, CO, June 2011.
- Khrulkov, V., Mirvakhobova, L., Ustinova, E., Oseledets, I., and Lempitsky, V. Hyperbolic image embeddings. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, June 2020.
- Kochurov, M., Karimov, R., and Kozlukov, S. Geoopt: Riemannian optimization in pytorch, 2020.
- Koller, D. and Sahami, M. Hierarchically classifying documents using very few words. Technical report, Stanford InfoLab, 1997.

- Krause, J., Stark, M., Deng, J., and Fei-Fei, L. 3d object representations for fine-grained categorization. In *4th International IEEE Workshop on 3D Representation and Recognition (3dRR-13)*, Sydney, Australia, 2013.
- Krizhevsky, A. Learning multiple layers of features from tiny images, 2009.
- Liu, Q., Nickel, M., and Kiela, D. Hyperbolic graph neural networks. In *Advances in Neural Information Processing Systems 32*, pp. 8230–8241, 2019.
- Liu, W., Wen, Y., Yu, Z., and Yang, M. Large-margin softmax loss for convolutional neural networks. In *Proceedings of the 33rd International Conference on International Conference on Machine Learning - Volume 48, ICML'16*, pp. 507–516. JMLR.org, 2016.
- McCallum, A., Rosenfeld, R., Mitchell, T. M., and Ng, A. Y. Improving text classification by shrinkage in a hierarchy of classes. In *ICML*, volume 98, pp. 359–367, 1998.
- Mikolov, T., Chen, K., Corrado, G., and Dean, J. Efficient estimation of word representations in vector space. *arXiv preprint arXiv:1301.3781*, 2013a.
- Mikolov, T., Sutskever, I., Chen, K., Corrado, G. S., and Dean, J. Distributed representations of words and phrases and their compositionality. In *Advances in neural information processing systems*, pp. 3111–3119, 2013b.
- Nickel, M. and Kiela, D. Poincaré embeddings for learning hierarchical representations. In *Advances in neural information processing systems*, pp. 6338–6347, 2017.
- Sela, Y., Freiman, M., Dery, E., Edrei, Y., Safadi, R., Pappo, O., Joskowicz, L., and Abramovitch, R. fmri-based hierarchical svm model for the classification and grading of liver fibrosis. *IEEE transactions on biomedical engineering*, 58(9):2574–2581, 2011.
- Shimizu, R., Mukuta, Y., and Harada, T. Hyperbolic neural networks++. In *International Conference on Learning Representations*, 2021.
- Skopek, O., Ganea, O.-E., and Bécigneul, G. Mixed-curvature variational autoencoders. *arXiv preprint arXiv:1911.08411*, 2019.
- Tifrea, A., Bécigneul, G., and Ganea, O.-E. Poincaré glove: Hyperbolic word embeddings. *arXiv preprint arXiv:1810.06546*, 2018.
- van der Maaten, L. and Hinton, G. Visualizing data using t-sne. *Journal of Machine Learning Research*, 9(86): 2579–2605, 2008.
- Vendrov, I., Kiros, R., Fidler, S., and Urtasun, R. Order-embeddings of images and language. In *4th International Conference on Learning Representations, ICLR 2016, San Juan, Puerto Rico, May 2-4, 2016, Conference Track Proceedings*, 2016.
- Wang, K., Zhou, S., and Liew, S. C. Building hierarchical classifiers using class proximity. In *VLDB*, volume 99, pp. 363–374. Citeseer, 1999.
- Weigend, A. S., Wiener, E. D., and Pedersen, J. O. Exploiting hierarchy in text categorization. *Information Retrieval*, 1(3):193–216, 1999.
- Welinder, P., Branson, S., Mita, T., Wah, C., Schroff, F., Belongie, S., and Perona, P. Caltech-UCSD Birds 200. Technical Report CNS-TR-2010-001, California Institute of Technology, 2010.
- Xie, P., Deng, Y., Zhou, Y., Kumar, A., Yu, Y., Zou, J., and Xing, E. P. Learning latent space models with angular constraints. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pp. 3799–3810. JMLR.org, 2017.
- Zhu, J.-Y., Krähenbühl, P., Shechtman, E., and Efros, A. A. Generative visual manipulation on the natural image manifold. In *European Conference on Computer Vision*, pp. 597–613. Springer, 2016.