

# A Survey of Learning on Small Data

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**Abstract**—Learning on big data brings success for artificial intelligence (AI), but the annotation and training costs are expensive. In future, learning on small data is one of the ultimate purposes of AI, which requires machines to recognize objectives and scenarios relying on small data as humans. A series of machine learning models is going on this way such as active learning, few-shot learning, deep clustering. However, there are few theoretical guarantees for their generalization performance. Moreover, most of their settings are passive, that is, the label distribution is explicitly controlled by one specified sampling scenario. This survey follows the agnostic active sampling under a PAC (Probably Approximately Correct) framework to analyze the generalization error and label complexity of learning on small data using a supervised and unsupervised fashion. With these theoretical analyses, we categorize the small data learning models from two geometric perspectives: the Euclidean and non-Euclidean (hyperbolic) mean representation, where their optimization solutions are also presented and discussed. Later, some potential learning scenarios that may benefit from small data learning are then summarized, and their potential learning scenarios are also analyzed. Finally, some challenging applications such as computer vision, natural language processing that may benefit from learning on small data are also surveyed.

**Index Terms**—Big data, artificial intelligence, small data, active learning, PAC framework, theoretical guarantee, hyperbolic geometry.

## 1 INTRODUCTION

“**T**HAT’S a cat sleeping in the bed, the boy is patting the elephant, those are people that are going on an airplane, that’s a big airplane...”. “This is a three-year child describing the pictures she sees” – said by Fei-Fei Li. She presented a famous lecture of “how we are teaching computers to understand pictures” in the Technology Entertainment Design (TED) 2015<sup>1</sup>. In the real world, humans can recognize objectives and scenarios only relying on one picture based on their prior knowledge. However, machines may need more. In the past few decades, artificial intelligence (AI) [1] [2] technology helped machines to be more intelligent like humans by learning on big data [3] [4]. By modeling the neuron propagation of the human brain, a series of expressive AI systems are built, *e.g.*, Deep Blue [5], AlphaGo [6].

Of course, the talent of AI is not innate. Training on big data helps AI to recognize different objectives and scenarios. To process big data, a set of techniques, *e.g.*, MapReduce [7], Hadoop [8], were implemented to access large-scale data, extracting useful information for AI decisions. Specifically, MapReduce is distributed across multiple heterogeneous clusters and Hadoop processes data through cloud providers. However, training and annotating large-scale data are quite expensive, although we adopt

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<sup>1</sup>[https://www.ted.com/talks/fei\\_fei\\_li\\_how\\_we\\_re\\_teaching\\_computers\\_to\\_understand\\_pictures?language=en](https://www.ted.com/talks/fei_fei_li_how_we_re_teaching_computers_to_understand_pictures?language=en)

those big data processing techniques.

“AI is not just for the big guys anymore<sup>2</sup>.” A novel perspective thinks the small data revolution is ongoing and training on small data with a desired performance is one of the ultimate purpose of AI. Technically, human experts expect to relieve the need on big data and find a new breakthrough for AI systems, especially for the configuration of the deep neural networks [9]. Related works including limited labels [10] [11], fewer labels [12] [13] [14], less data [15] [16], *etc.*, were already realized by those low-resource deep learning researchers. Formally, few-shot learning [17], which is referred to as low-resource learning, is a unified topic which studies small data with limited information. Based on Wang *et al.*’s survey [18], an explicit scenario of few-shot learning is feature generation [19], that is, generating artificial features by the given limited or insufficient information. Another scenario with implicit supervision information is more challenging, which relies on retraining the learning model [19] [20] with those highly-informative examples, such as private data. Theoretically, most of the few-shot learning scenarios are passive, that is, the label distribution is explicitly controlled by one specified sampling scenario. Thence, active learning [21] attracts our eyes where the label acquisitions are controlled by a learning algorithm or humans.

Different from few-shot learning, the annotation scenario of active learning is not so limited. One active learning algorithm can stop its iterative sampling at anytime due to desired algorithm performance or exhausted annotation budget. There are two categories for active learning: active sampling theory over hypothesis class [22] and active sampling algorithm over realized scenarios [23], where the theory studies present the label complexity and convergence guarantees for those algorithmic paradigms. The typical theoretical analyses are derived from a PAC ((Probably Approximately Correct)) [24] style, which aims at an agnostic setting such as [25]. To control the active sampling, there is one

<sup>2</sup><https://www.forbes.com/sites/forbestechcouncil/2020/05/19/the-small-data-revolution-ai-isnt-just-for-the-big-guys-anymore/?sh=4b8d35c82bbb>

kind of error disagreement coefficient that searches a target data, which can maximize the hypothesis update the most, where those updates are required to be positive and helpful. Therefore, the active sampling also is a hypothesis-pruning [26] process, which tries to find the optimal hypothesis from a given hypothesis class, where the hypotheses are maintained from a version space [27] [28] over the decision boundaries [29] of classes. Geometrically, the version space of an enclosed class is usually embedded in a tube structure [30] [31] which has a homeomorphic topology as with the assumed spherical class.

### 1.1 Motivations and Contributions

Learning on small data is essential for advancing AI. As a preemptive topic, few-shot learning presented exploration for limited data training. However, the setting of few-shot learning is a passive scenario, which stipulates insufficient label information by the task itself. Meanwhile, there are few theoretical guarantees for its generalization performance. This motivates us to give theoretical analysis for learning on small data. With active sampling theory, we follow the PAC framework to present a set of error and label complexity bounds for learning on small data. To summarize those algorithmic paradigms, we then categorize the small data learning models into: the Euclidean and hyperbolic (non-Euclidean) representation including their deep learning scenarios. Concretely, contributions of this survey are summarized as follows.

- We present a formal definition for learning on small data. The definition is a model-agnostic setting that derives a more general concept from a machine learning perspective.
- From a PAC perspective, we are the first to present theoretical guarantees for learning on small data via active sampling theory. The generalization error and label complexity bounds of learning on small data are presented.
- From a geometric perspective, we divide the small data learning models into two categories: the Euclidean and hyperbolic representation, where their optimization solvers are analyzed.
- We investigate some new directions of learning on small data for potential learning scenarios and real-world challenging applications.

### 1.2 PAC Framework of This Survey

In 1984, Leslie Valiant proposed a computational learning concept-Probably Approximately Correct (PAC) [32], which presents mathematical analysis for machine learning under fixed distribution and parameter assumptions. Theoretically, the learner is required to select a generalization hypothesis (also called conceptual function) from a candidate hypothesis class by observing those received data and labels. The goal is to converge the hypothesis into approximately correct generalization, which properly describes the probability distribution of the unseen samples. One key content of PAC leaning is to derive the computational complexity bounds such as sample complexity [33], generalization errors, Vapnik–Chervonenki(VC) dimension [34].

In computational learning theory, active learning tries to prune the candidate infinite concept class into the optimal hypothesis, which keeps consistent properties as with its labeled examples [22]. The main difference to typical PAC learning is that the active learning controls the hypothesis-pruning by receiving fewer training data. Therefore, active learning that finds hypotheses

consistent with a small set of labeled examples, can be deemed as a standard hypothesis-pruning to PAC learning. With this framework, we present this survey.

### 1.3 Organization of The Survey

The remainder of this survey is organized as follows. Section 2 presents the related literature of learning on small data including the few-shot learning and active learning. Section 3 presents a formal definition on learning on small data and presents its PAC analysis including the label complexity and generalization error bounds. From a geometric perspective, Section 4 introduces the Euclidean and non-Euclidean paradigms for learning on small data, and Section 5 presents related optimization solvers. Later, Section 6 discusses the potential scenarios of learning on small data representation, and Section 7 presents their challenging scenarios. Then, Section 8 presents some interesting applications about small data. Section 9 finally concludes this survey.

## 2 FEW-SHOT LEARNING VS. ACTIVE LEARNING

Few-shot learning could be considered as a preemptive topic of learning on small data with passive scenario. Differently, active learning also presents solutions for small data, but with an active sampling scenario.

### 2.1 Few-shot Learning

Finding the optimal hypothesis consistent with the full training set is a standard theoretical description of machine learning to PAC. The convergence process is to perform hypothesis-pruning in the candidate hypothesis class. Therefore, the number of the hypotheses of a fixed geometric region determines the volume of the hypothesis space, which affects the speed and cost of hypothesis-pruning.

Given a full training set  $\mathcal{X}$  with  $n$  samples, let  $\mathcal{H}$  be the hypothesis class, the VC dimension bound of  $\mathcal{H}$  can be used to describe the complexity of the convergence difficulty of the hypothesis-pruning for a given learning algorithm. We thus follow the agnostic active learning [25] to define  $N(\mathcal{H}, n, k, \mathcal{A})$  as a class of function which controls the convergence of the learning algorithm  $\mathcal{A}$  in hypothesis class  $\mathcal{H}$ , associating from  $n$  training samples with  $k$  classes.

**Definition 1.** *Machine learning. From a hypothesis-pruning perspective, given any machine learning algorithm  $\mathcal{A}$ , its candidate hypothesis class is characterized by  $\mathcal{H}$ , which satisfies 1) a VC dimension bound of  $\mathcal{O}(2^n)$ , and 2) a safety uniform bound of pruning into a non-null hypothesis is  $N(\mathcal{H}, n, k, \mathcal{A}) \geq \mathcal{O}(\frac{k-1}{k}n)$ , and 3) the VC dimension bound of a non-null hypothesis subspace is  $\mathcal{O}(2^n - 2^{\frac{(k-1)n}{k}})$ .*

Note that the uniform bound aims at an expected complexity and a non-null hypothesis requires the training examples to cover all label categories. Given any class has at least  $\eta$  data, a safety guarantee requires  $N(\mathcal{H}, n, k, \mathcal{A}) \geq \mathcal{O}(n - \eta)$ . For a uniform estimation on  $\eta \approx \mathcal{O}(\frac{n}{k})$  over all possibilities of  $\eta = 1, 2, 3, \dots, \frac{n}{k}$ , a safety uniform bound of pruning into a non-null hypothesis is  $\mathcal{O}(\frac{k-1}{k}n)$ .

Assume that  $\eta \ll \frac{n}{k}$ , the typical machine learning scenario becomes a few-shot learning process.

**Definition 2.** *Few-shot learning. From a hypothesis-pruning perspective, given any few-shot learning algorithm  $\mathcal{A}$ , its candidate*

*hypothesis class is characterized by  $\mathcal{H}$ , which satisfies 1) a VC dimension bound of  $\mathcal{O}(2^n)$ , 2) a safety uniform bound of pruning into a non-null hypothesis is  $N(\mathcal{H}, n, k, \mathcal{A}) \geq \mathcal{O}(n - \eta)$ , and 3) a VC dimension bound of shrinking into a non-null hypothesis subspace is  $\mathcal{O}(2^n - 2^{n-\eta})$ , where  $2^n - 2^{n-\eta} \gg \frac{k-1}{k}n$ .*

From Definition 2, few-shot learning can be deemed as a special case of typical machine learning with limited supervision information. One important characteristics of it is its tighter volume of the non-null hypothesis space since  $\mathcal{O}(2^n - 2^{n-\eta}) \gg \mathcal{O}(\frac{k-1}{k}n)$ . Therefore, compared with typical machine learning, any few-shot learning algorithm will result in looser safety bound to prune into a non-hypothesis.

In realizable settings, one typical few-shot learning scenario is feature generation [19] via model retraining. In this scenario, the learning algorithm generates handwritten features like humans by pre-training the model with prior knowledge, where the retaining will not stop, until a desired performance is achieved. However, retraining the learning model is adopted in rare cases, which cannot properly generate highly-trust features. For example, one special case of few-shot learning is one-shot learning [35] which relies on only one data in some classes; the other more extreme case is zero-shot learning [36] where some classes don not include any data or labels. Their detailed definitions are presented as follows.

**Definition 3.** *One-shot learning. From a hypothesis-pruning perspective, given any one-shot learning algorithm  $\mathcal{A}$ , its candidate hypothesis class is characterized by  $\mathcal{H}$ , which satisfies 1) a VC dimension bound of  $\mathcal{O}(2^n)$ , 2) a safety uniform bound of pruning into a non-null hypothesis is  $N(\mathcal{H}, n, k, \mathcal{A}) \geq \mathcal{O}(n)$ , and 3) the VC dimension bound of shrinking into a non-null hypothesis subspace is  $\mathcal{O}(2^n)$ .*

**Definition 4.** *Zero-shot learning. From a hypothesis-pruning perspective, given any zero-shot learning algorithm  $\mathcal{A}$ , its candidate hypothesis class is characterized by  $\mathcal{H}$ , which satisfies 1) a VC dimension bound of  $\mathcal{O}(2^n)$ , 2) an inapplicable safety uniform bound of pruning into a non-null hypothesis, and 3) an inapplicable VC dimension bound of shrinking into a non-null hypothesis subspace.*

Usually, the few-shot learning is also related to weakly-supervised learning [37] [38], which includes incomplete, inaccurate, noisy, and outlier information, etc. From this perspective, few-shot learning can be considered as one special setting of weakly-supervised learning with incomplete label information. Imbalanced learning [39], transfer learning [40], meta-learning [41], etc., also have inherent connections with few-shot learning. However, there are no theoretical analyses for the convergence of the optimal hypothesis.

## 2.2 Active Learning

Active learning prunes the candidate hypothesis class into a desired convergence. The pruning process usually is to zoom out [42] the hypothesis space by querying those highly-informative updates. Therefore, the assumption of active learning requires any update from the hypothesis-pruning should be non-null. Here we present the definition on active learning.

**Definition 5.** *Active learning. From a hypothesis-pruning perspective, given any active learning algorithm  $\mathcal{A}$  with a querying budget  $\mathcal{Q}$ , its candidate hypothesis class is characterized by  $\mathcal{H}$ , which satisfies 1) a VC dimension bound of  $\mathcal{O}(2^n)$ , 2) a safety*

*uniform bound of pruning into a non-null hypothesis is  $\mathcal{O}(1)$ , and 3) the VC dimension bound of a non-null hypothesis subspace is  $\mathcal{O}(2^{\mathcal{Q}})$ .*

Note that active learning requires the updates of hypotheses are positive and non-null. Any subsequent hypotheses can converge into a safety state, which derives a safety uniform bound of  $\mathcal{O}(1)$ . Different from few-shot learning, the scenario of active learning is controlled by humans, which always keep a non-null update on hypotheses. It is thus that its VC dimension bound is tighter than the typical machine learning and few-shot learning. To find feasible hypothesis updates, active learning always uses an error disagreement coefficient [43] to control the hypothesis-pruning.

**Error disagreement.** Given a finite hypothesis class  $\mathcal{H}$ , active learning iteratively updates the current hypothesis  $h_{\mathcal{Q}} \in \mathcal{H}$  at  $t$ -time into the optimal hypothesis  $h^* \in \mathcal{H}$ . Let an active learning algorithm  $\mathcal{A}$  perform  $\mathcal{Q}$  rounds of querying from  $\mathcal{X}$ , assume that  $\ell(\cdot, \cdot)$  denotes the loss of mapping  $\mathcal{X}$  into  $\mathcal{Y}$  with multi-class setting, we define the total loss of the  $\mathcal{Q}$  rounds of querying as  $R(h_{\mathcal{Q}}) = \sum_{i=1}^{\mathcal{Q}} \frac{q_t}{p_i} \ell(h(x_t), y_t)$ , where  $y_t$  denotes the label of  $x_t$ ,  $q_t$  satisfies the Bernoulli distribution of  $q_t \in \{0, 1\}$ , and  $\frac{1}{p_i}$  denotes the weight of sampling  $x_t$ . On this setting, the sampling process then adopts an error disagreement to control the hypothesis updates:

$$\theta_{\mathcal{A}} = \mathbb{E}_{x_t \in \mathcal{D}} \sup_{h \in B(h^*, r)} \left\{ \frac{\ell(h(x_t), \mathcal{Y}) - \ell(h^*(x_t), \mathcal{Y})}{r} \right\}, \quad (1)$$

where  $\mathcal{D}$  denotes the margin distribution over  $\mathcal{X}$ , drawing the candidate hypotheses. To reduce the complexity of the pruning process, one can shrink  $\mathcal{D}$  from the marginal distribution of  $\mathcal{X}$ , which derives the most of hypotheses, such as [25], [44].

Correspondingly,  $\ell(h(x), h'(x))$  denotes the hypothesis disagreement of  $h$  and  $h'$ , which can be specified as the best-in-class error on  $\mathcal{Y}$

$$\ell(h(x), h'(x)) = \left| \max_{y \in \mathcal{Y}} \ell(h(x), y) - \ell(h'(x), y) \right|, \quad (2)$$

where  $y \in \mathcal{Y}$ , and  $\ell(h(x), h'(x))$  also can be simply written as  $\ell(h, h')$ . Once the hypothesis update w.r.t. error after adding  $x_t$  is larger than  $\theta_{\mathcal{A}}$ , the active learning algorithm  $\mathcal{A}$  solicits  $x_t$  as a significant update. Besides Eq. (2),  $\ell(h(x), h'(x))$  also can be specified as all-in-class error [45], error entropy [46], etc.

## 3 APPROXIMATELY GENERALIZATION ANALYSIS

From a hypothesis-pruning perspective, we firstly present a more general concept for learning on small data. Then, we present the generalization analysis of the convergence of the optimal hypothesis on error and label complexity bounds under a supervised and unsupervised fashion, respectively.

### 3.1 A More General Concept

For agnostic sampling, any hypothesis  $h \in \mathcal{H}$  can achieve a generalization error of  $\text{err}(h)$ . With a probability at least  $1 - \delta$ , after  $\mathcal{Q}$  times of sampling, if  $\text{err}(h)$  converges into its optimal error, based on Theorem 1 of [25], there exists an upper bound of  $\text{err}(h) + c \left( \frac{1}{\mathcal{Q}} (\text{dlog } \mathcal{Q} + \log \frac{1}{\delta}) + \sqrt{\frac{\text{err}(h)}{\mathcal{Q}}} \mathcal{Q} (\text{dlog } \mathcal{Q} + \log \frac{1}{\delta}) \right)$ . By relaxing the constant  $c$  and  $\text{err}(h)$  ( $\text{err}(h) < 1$ ), the label complexity of any learning algorithm satisfies an upper bound of

$$N(\mathcal{H}, n, \mathcal{Q}, \mathcal{A}) \leq \mathcal{O} \left( \frac{1}{\mathcal{Q}} (\text{dlog } \mathcal{Q} + \log \frac{1}{\delta}) \right). \quad (3)$$

Eq. (3) presents a coarse-grained observation on the upper bound of the label complexity. We next introduce the error disagreement coefficient  $\theta_{\mathcal{A}}$  to prune the hypothesis class. If the learning algorithm controls the hypothesis updates by Eq. (1), based on Theorem 2 of [25], the expected label cost for the convergence of  $err(h)$  is at most  $1 + c\theta_{\mathcal{A}} \left( d\log Q + \log \frac{1}{\delta} \right) \log Q$ . By relaxing the constant  $c$ , we have

$$N(\mathcal{H}, n, Q, \mathcal{A}) \leq \mathcal{O}\left(\theta_{\mathcal{A}} \left( d\log Q + \log \frac{1}{\delta} \right) \log Q\right). \quad (4)$$

With the inequalities of Eqs. (3) and (4), we present a more general concept for small data.

**Definition 6.** *Small data. With standard empirical risk minimization, learning small data from  $\mathcal{D}$  over  $Q$  times of sampling satisfies an incremental update on the optimal hypothesis with an error of  $err(h^*)$ ,*

$$\begin{aligned} \arg \min_Q err(h_Q) &\leq \left( err(h^*) + \mathcal{O}\left(\sqrt{err(h^*)\Omega} + \Omega\right) \right) \\ \text{s.t. } \Omega &= \frac{d\log Q + \log \frac{1}{\delta}}{Q}, \end{aligned} \quad (5)$$

where  $h_Q$  denotes the updated hypothesis at the  $Q$ -time of sampling.

### 3.2 Learning on Small Data

With the standard definition on small data, we next study that how to learn small data via empirical risk minimization (ERM), which can be generalized into different loss functions in real-world models. Our main theorem of the label complexity in regard to ERM is then presented in Theorems 1 and 2.

Before presenting Theorem 1, we need a technical lemma about the importance-weighted empirical risk minimization on  $\ell(h_Q, h^*)$ . The involved techniques refer to the Corollary 4.2 of J. Langford *et al.*'s work in [47], and the Theorem 1 of C. Sahyoun *et al.*'s work [48].

**Lemma 1.** *Let  $R(h)$  be the expected loss (also called learning risk) that stipulates  $R(h) = \mathbb{E}_{x \sim \mathcal{D}}[\ell(h(x), y)]$ , and  $R(h^*)$  be its minimizer. On this setting,  $\ell(h_Q, h^*)$  then can be bounded by  $\ell(h_Q, h^*) \leq R(h_Q) - R(h^*)$  that stipulates  $\mathcal{H}_Q := \{h \in \mathcal{H}_{Q-1} : R(h_Q) \leq R(h^*) + 2\Delta_{Q-1}\}$ , where  $\Delta_{Q-1}$  adopts a form [49] of*

$$\frac{1}{Q-1} \left[ \sqrt{\left[ \sum_{s=1}^{Q-1} p_s \right] \log \left[ \frac{(Q-1)|\mathcal{H}|}{\delta} \right]} + \log \left[ \frac{(Q-1)|\mathcal{H}|}{\delta} \right] \right],$$

where  $|\mathcal{H}|$  denotes the number of hypothesis in  $\mathcal{H}$ , and  $\delta$  denotes a probability threshold requiring  $\delta > 0$ . Since  $\sum_{s=1}^{Q-1} p_s \leq Q-1$ ,  $\Delta_{Q-1}$  can then be bounded by

$$\Delta_{Q-1} = \sqrt{\left( \frac{2}{Q-1} \right) \log \left( 2Q(Q-1) \right) \frac{|\mathcal{H}|^2}{\delta}},$$

which denotes the loss disagreement bound to approximate a desired target hypothesis such that  $R(h_Q) - R(h^*) \leq 2\Delta_{Q-1}$ .

There are two fashions to learn small data including supervised and unsupervised learning. We next present their different generalization analyses.

#### 3.2.1 Supervised Fashion

We follow the setting of Lemma 1 to present the learning risk and label complexity for learning on small data under  $Q$  rounds of importance sampling.

**Theorem 1.** *Given  $Q$  rounds of querying by employing the active learning algorithm  $\mathcal{A}$ , with a probability at least  $1 - \delta$ , for all  $\delta > 0$ , for any  $Q > 0$ , the error disagreement of  $R(h_Q)$  and  $R(h^*)$  of learning on small data is bounded by*

$$\begin{aligned} &R(h_Q) - R(h^*) \\ &\leq \max_Q \left\{ \frac{2}{Q} \left[ \sqrt{\sum_{t=1}^Q p_t} + 6\sqrt{\log \left[ \frac{2(3+Q)Q^2}{\delta} \right]} \right] \right. \\ &\quad \times \left. \sqrt{\log \left[ \frac{16Q^2|\mathcal{H}_i|^2 \log Q}{\delta} \right]} \right\}, \end{aligned}$$

Then, with a probability at least  $1 - 2\delta$ , for all  $\delta > 0$ , the label complexity of learning on small data can be bounded by

$$\begin{aligned} N(\mathcal{H}, n, Q, \mathcal{A}) &\leq \max_Q K_\ell \left\{ \left[ \sum_{j=1}^Q \theta_{\mathcal{A}} R_j^* Q p_j \right] \right. \\ &\quad \left. + \sum_{j=1}^Q O\left(\sqrt{R_j^* Q p_j \log \left[ \frac{Q|\mathcal{H}_i|Q}{\delta} \right]}\right) + O\left(Q \log^3 \left( \frac{\tau |\mathcal{H}_i| Q}{\delta} \right)\right) \right\}. \end{aligned}$$

where  $K_\ell$  is the slope asymmetry over the loss  $\ell$ ,  $K_\ell = \sup_{x'_t, x_t \in \mathcal{D}} \left| \frac{\max \ell(h(x_t), \mathcal{Y}) - \ell(h(x'_t), \mathcal{Y})}{\min \ell(h(x_t), \mathcal{Y}) - \ell(h(x'_t), \mathcal{Y})} \right|$ ,  $R_j^*$  denotes the best-in-class risk at  $j$ -time querying, and  $|\mathcal{H}|$  denotes the element number of  $\mathcal{H}$ .

The proofs of Theorem 1 and 2 of [49] can be adopted to prove the two inequalities of Theorem 1, respectively.

#### 3.2.2 Unsupervised Fashion

By employing unsupervised learning, the learning risk and label complexity of Theorem 1 are degenerated into a polynomial expression [50].

Given the input dataset  $\mathcal{X}$  with  $n$  samples, it is divided into  $k$  clusters:  $\{\mathcal{B}_1, \mathcal{B}_2, \dots, \mathcal{B}_k\}$ , where  $\mathcal{B}_i$  has  $N_i$  samples. Learning small data performs IWAL for any  $\mathcal{B}_i$ . Specifically, it employs a new error disagreement  $\theta_{LSD}$  to control the hypothesis updates:

$$\theta_{LSD} = \mathbb{E}_{x_t \in \mathcal{B}_i} \sup_{h \in B(h^*, r)} \left\{ \frac{\ell(h(x_t), \mathcal{Y}) - \ell(h^*(x_t), \mathcal{Y})}{r} \right\}. \quad (6)$$

**Theorem 2.** *Given  $T$  rounds of querying by employing the active learning algorithm  $\mathcal{A}$ , let  $Q$  be the number of ground-truth queries. If learning small data performs  $\mathcal{A}$  for any  $\mathcal{B}_i$ , each cluster will have  $\tau = T/k$  rounds of querying. Then, with a probability at least  $1 - \delta$ , for all  $\delta > 0$ , for any  $Q > 0$ , the error disagreement of  $R(h_\tau)$  and  $R(h^*)$  of learning on small data is bounded by  $k$  times of polynomial*

$$\begin{aligned} &R(h_\tau) - R(h^*) \\ &\leq k \times \max_{\mathcal{H}_i, i=1, 2, \dots, k} \left\{ \frac{2}{\tau} \left[ \sqrt{\sum_{t=1}^\tau p_t} + 6\sqrt{\log \left[ \frac{2(3+\tau)\tau^2}{\delta} \right]} \right] \right. \\ &\quad \times \left. \sqrt{\log \left[ \frac{16\tau^2|\mathcal{H}_i|^2 \log \tau}{\delta} \right]} \right\}, \end{aligned}$$

Then, with a probability at least  $1 - 2\delta$ , for all  $\delta > 0$ , the label complexity of learning on small data can be bounded by

$$\begin{aligned} N(\mathcal{H}, n, \mathcal{Q}, \mathcal{A}) \\ \leq 8k \times \max_{\mathcal{H}_i, i=1,2,\dots,k} K_\ell \left\{ \left[ \sum_{j=1}^{N_i} \theta_{\text{LSD}} R_j^* \tau p_j \right] \right. \\ \left. + \sum_{j=1}^{N_i} O\left( \sqrt{R_j^* \tau p_j \log\left[\frac{\tau|\mathcal{H}_i|N_i}{\delta}\right]} \right) + O\left( N_i \log^3\left(\frac{\tau|\mathcal{H}_i|N_i}{\delta}\right) \right) \right\}. \end{aligned}$$

where  $K_\ell$  is the slope asymmetry over the limited loss  $\ell$  on  $\mathcal{B}_i$ , i.e.,  $\ell_{\mathcal{B}_i}$ ,  $K_\ell = \sup_{x'_t, x_t \in \mathcal{B}_i} \left| \frac{\max \ell_{\mathcal{B}_i}(h(x_t), \mathcal{Y}) - \ell_{\mathcal{B}_i}(h(x'_t), \mathcal{Y})}{\min \ell_{\mathcal{B}_i}(h(x_t), \mathcal{Y}) - \ell_{\mathcal{B}_i}(h(x'_t), \mathcal{Y})} \right|$ ,  $R_j^*$  denotes the best-in-class risk at  $j$ -time querying, and  $|\mathcal{H}|$  denotes the element number of  $\mathcal{H}$ . More details and proofs are presented in Appendix.Part A.

## 4 A GEOMETRIC PERSPECTIVE

From a geometric perspective, learning on small data could be performed in the Euclidean and non-Euclidean (hyperbolic) space. To learn effective geometric representation, we investigate the properties of the Euclidean and hyperbolic mean with respect to the unified expression of Fréchet mean [51].

### 4.1 Fréchet Mean

To understand a collection of observations sampled from a statistical population, the *mean* of observations is adopted as one powerful statistics to summarize the observations from an underlying distribution. What does *mean* mean? It may vary under different data distributions and depend on the goal of the statistics. To characterize the representation of real-world data, typical candidates for mean may be the arithmetic mean and the median, but in some cases, the geometric or harmonic mean may be preferable. When the data exists in a set without a vector structure, such as a manifold or a metric space, a different concept of *mean* is required, i.e., Fréchet mean [52].

**Fréchet mean on probability measures.** We explore a general mean that can be defined with less structure but encompasses the common notions of *mean* – the *Fréchet mean*. The Fréchet mean is an important entailment (implication) in geometric representations, that embeds a “centroid” to indicate its local features (neighbors) on a metric space. For a distance space  $(\mathcal{X}, d_{\mathcal{X}})$ , let  $\mathbb{P}$  be a probability measure on  $\mathcal{X}$  with  $\int d_{\mathcal{X}}^2(x, y) d\mathbb{P}(x) < \infty$  for all  $y \in \mathcal{X}$ , the Fréchet mean is to operate the argmin optimization [51] of

$$\mu_{\mathcal{X}} = \arg \min_{\mu \in \mathcal{X}} \int d_{\mathcal{X}}^2(x, \mu) d\mathbb{P}(x). \quad (7)$$

The Fréchet means defined by the probability measures is more generalized and can be derived to more common objects.

**Advantages of Fréchet mean.** The Fréchet mean w.r.t. Eq. (7) has two significant advantages [51]. 1) It provides a common construction for many well-known notions of *mean* in machine learning and thus implies many interesting properties of data. 2) It provides the notion of *mean* in spaces with less structure than Euclidean spaces, e.g., metric spaces or Riemannian manifolds, thus widening the possibility of adopting machine learning methods in these spaces.

**Fréchet mean on Riemannian manifold.** We next observe the Fréchet mean on manifold. For an arbitrary Riemannian manifold  $\mathcal{M}$  with metric  $g_x(\cdot, \cdot)$  that projects the tangent space

$\mathcal{T}_x \mathcal{M} \times \mathcal{T}_x \mathcal{M} \rightarrow \mathbb{R}^n$  where  $\|v\|_g = \sqrt{g_x(v, v)}$ , let  $\gamma(t) : [a, b] \rightarrow \mathcal{M}$  be a geodesics that stipulates distance  $d_{\mathcal{M}}(\cdot, \cdot)$  as the integral of the first order of the geodesics. For all  $x, y \in \mathcal{M}$ , the distance  $d_{\mathcal{M}}(x, y) := \inf \int_a^b \|\gamma'(t)\|_g dt$  where  $\gamma(t)$  denotes any geodesics such that  $\gamma(a) = x, \gamma(b) = y$ . Given a point set  $\mathcal{X} = \{x_1, x_2, \dots, x_m\} \subseteq \mathcal{M}$  and set the probability density of each point  $x_i \in \mathcal{X}$  as  $\frac{1}{m}$ , the *weighted Fréchet mean* [51] is to operate the argmin optimization of

$$\mu_{\mathcal{M}} = \arg \min_{\mu \in \mathcal{M}} \sum_{i=1}^m \omega_i d_{\mathcal{M}}^2(x_i, \mu), \quad (8)$$

where  $\omega_i$  denotes the weight of  $x_i$ , and the constraint of  $\mu \in \mathcal{M}$  stipulates that  $\mu$  may converge in  $\mathcal{M}$  with infinite candidates. Given  $d_{\mathcal{M}}(a, b) := \|a - b\|_2$  defined in Euclidean geometry and  $\omega_i = 1/m$  for all  $i$ , the weighted Fréchet mean is then simplified into the Euclidean mean, which results in a fast computational time. This specified setting achieved promising results in the  $k$ -means clustering, maximum mean discrepancy optimization [53], etc.

### 4.2 Euclidean Mean

The Euclidean mean is the most widely adopted *mean* in machine learning. Meanwhile, the Euclidean mean is of great importance to perform aggregation operations such as attention [54], batch normalization [55]. Let  $\mathcal{R}^n$  denote the Euclidean manifold with zero curvature, and the corresponding Euclidean metric of which is defined as  $g^E = \text{diag}([1, 1, \dots, 1])$ . For  $\mathbf{x}, \mathbf{y} \in \mathcal{R}^n$ , the Euclidean distance is given as:

$$d_{\mathcal{R}}(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2. \quad (9)$$

Then  $(\mathcal{R}^n, d_{\mathcal{R}})$  is a complete distance space. We next present a formal description of Euclidean mean [56] based on the weighted Fréchet mean w.r.t. Eq. (8).

**Proposition 1.** Given a set of points  $\mathcal{X} = \{x_1, x_2, \dots, x_m\} \subseteq \mathcal{R}^n$ , the Euclidean mean  $\mu_{\mathcal{R}}$  minimizes the following problem:

$$\min_{\mu \in \mathcal{R}^n} \sum_{i=1}^m \omega_i d_{\mathcal{R}}^2(x_i, \mu), \quad (10)$$

where  $\omega_i \geq 0$  denotes the weight coefficient of  $x_i$ .

The completeness of  $(\mathcal{R}^n, d_{\mathcal{R}})$  guarantees that Eq. (10) has a closed gradient, so a unique solution exists. With Proposition 1, the Euclidean mean  $\mu_{\mathcal{R}}$  is unique with the closed-form solution of

$$\mu_{\mathcal{R}} = \frac{1}{m} \sum_{i=1}^m x_i. \quad (11)$$

### 4.3 Non-Euclidean Mean

Recent studies demonstrate that hyperbolic geometry has stronger expressive capacity than the Euclidean geometry to model hierarchical features [57], [58]. Meanwhile, the Euclidean mean extends naturally to the Fréchet mean on hyperbolic geometry. Next, we discuss the Fréchet mean on the Poincaré and Lorentzian model with respect to Riemannian manifold. The illustrations of Poincaré and Lorentz model are presented in Figure 1.

#### 4.3.1 Poincaré Centroid

The Poincaré ball model  $\mathcal{P}^n$  with constant negative curvature corresponds to the Riemannian manifold  $(\mathcal{P}^n, g_x^{\mathcal{P}})$ , where  $\mathcal{P}^n =$

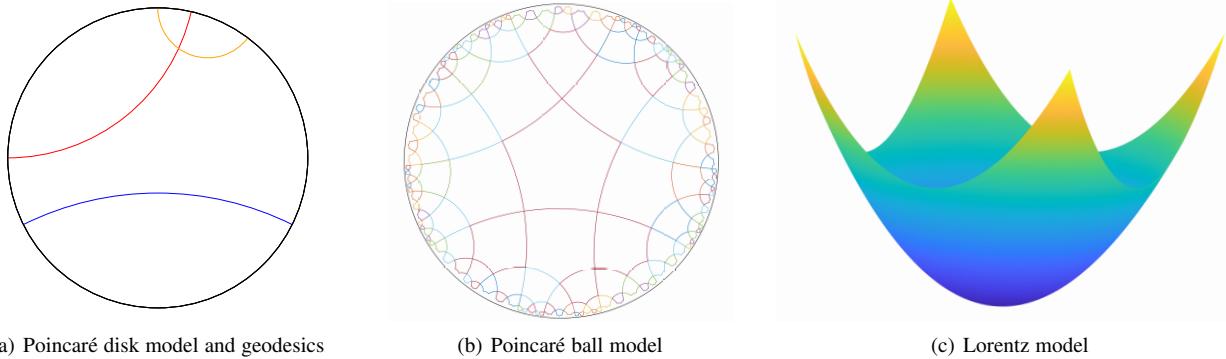


Figure 1: Illustration of Poincaré model and Lorentz model. (a) Poincaré disk model and geodesics. (b) Poincaré ball model (2D Poincaré ball model) and geodesics. Poincaré disk model is an open unit circle and all of its geodesics are perpendicular to the boundary. (b) Poincaré ball model is an open unit ball. The closer two points inside the model are to the boundary, the more the distance between them grows infinitely. (c) Lorentz model. It is defined as the upper sheet of a two-sheeted n-dimensional hyperboloid.

$\{x \in \mathbb{R}^n : \|x\| < 1\}$  denotes an open unit ball defined as the set of  $n$ -dimensional vectors whose Euclidean norm are smaller than 1. The Poincaré metric is defined as  $g_x^P = \lambda_x^2 g^E$ , where  $\lambda_x = \frac{2}{1-\|x\|^2}$  denotes the conformal factor and  $g^E$  denotes the Euclidean metric. For any  $\mathbf{x}, \mathbf{y}$  in  $\mathcal{P}^n$ , the Poincaré distance is given as [59]:

$$d_P(\mathbf{x}, \mathbf{y}) = \cosh^{-1} \left( 1 + 2 \frac{\|\mathbf{x} - \mathbf{y}\|^2}{(1 - \|\mathbf{x}\|^2)(1 - \|\mathbf{y}\|^2)} \right). \quad (12)$$

Then  $(\mathcal{P}^n, d_P)$  is a distance space. We thus have the following proposition for the Poincaré centroid [59] based on the Poincaré distance.

**Proposition 2.** Given a set of points  $\mathcal{X} = \{x_1, x_2, \dots, x_m\} \subseteq \mathcal{P}^n$ , the Poincaré centroid  $\mu_P$  minimizes the following problem:

$$\min_{\mu \in \mathcal{P}^n} \sum_{i=1}^m \omega_i d_P^2(x_i, \mu), \quad (13)$$

where  $\omega_i \geq 0$  denotes the weight coefficient of  $x_i$ .

There is no closed-form solution for the Poincaré centroid  $\mu_P$ , so Nickel *et al.* [59] computes it via gradient descent.

#### 4.3.2 Lorentzian Centroid

**Lorentz Model.** The Lorentz model  $\mathcal{L}^n$  with constant curvature  $-1/K$  avoids numerical instabilities that arise from the fraction in the Poincaré metric, for  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{n+1}$ , the Lorentzian scalar product is formulated as [60]:

$$\langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}} = -x_0 y_0 + \sum_{i=1}^n x_i y_i \leq -K. \quad (14)$$

This model of  $n$ -dimensional hyperbolic space corresponds to the Riemannian manifold  $(\mathcal{L}, g_{\mathcal{L}})$ , where  $\mathcal{L} = \{\mathbf{x} \in \mathbb{R}^{n+1} : \langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}} = -K, x_0 > 0\}$  (*i.e.*, the upper sheet of a two-sheeted  $n$ -dimensional hyperboloid) and  $g_{\mathcal{L}} = \text{diag}([-1, 1, \dots, 1])$  denotes the Lorentz metric. The squared Lorentz distance for  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{n+1}$  which satisfies all the axioms of a distance other than the triangle inequality is defined as [60]:

$$d_{\mathcal{L}}^2(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_{\mathcal{L}}^2 = -2K - 2 \langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}}. \quad (15)$$

Proposition 3 presents Lorentz centroid that represents the aspherical distributions under a Lorentz model [60].

**Proposition 3.** Given a set of points  $\mathcal{X} = \{x_1, x_2, \dots, x_m\} \subseteq \mathcal{L}^n$ , the Lorentzian centroid  $\mu_{\mathcal{L}}$  minimizes the following problem:

$$\min_{\mu \in \mathcal{L}^n} \sum_{i=1}^m \omega_i d_{\mathcal{L}}^2(x_i, \mu), \quad (16)$$

where  $\omega_i \geq 0$  denotes the weight coefficient of  $x_i$ .

The Lorentzian centroid  $\mu_{\mathcal{L}}$  is unique with the closed-form solution of

$$\mu_{\mathcal{L}} = \sqrt{K} \frac{\sum_{i=1}^m \omega_i x_i}{\|\sum_{i=1}^m \omega_i x_i\|_{\mathcal{L}}}, \quad (17)$$

where  $\|\mathbf{a}\|_{\mathcal{L}} = \sqrt{\|\mathbf{a}\|_{\mathcal{L}}^2}$  denotes the modulus of the imaginary Lorentzian norm of the positive time-like vector  $\mathbf{a}$ .

#### 4.3.3 Lorentzian Focal Point

With [61], the Euclidean norm of Lorentz centroid  $\mu_{\mathcal{L}}$  decreases, thus yielding an effective approximation to the focal point which is more representative than Lorentz centroid for the aspherical distributions. However, the approximation cannot only depend on  $K$  due to uncertain parameter perturbations. We should also control the coefficient  $\omega_i$  to approximate the Lorentzian focal point. Here  $\omega_i$  w.r.t. Eq. (17) can be written as [61]:

$$\omega_i = \frac{d_{\mathcal{L}}^2(x_i, \mu)}{\sum_{i=1}^m d_{\mathcal{L}}^2(x_i, \mu)}, \quad (18)$$

Then we present the approximation of Lorentzian focal point in Proposition 4 [61].

**Proposition 4.** Given a set of points  $\mathcal{X} = \{x_1, x_2, \dots, x_m\} \subseteq \mathcal{L}^n$ , the Lorentzian focal point  $\mu_{\mathcal{F}}$  minimizes the following problem:

$$\min_{\mu \in \mathcal{L}^n} \sum_{i=1}^m \omega_i \langle x_i, \mu \rangle_{\mathcal{L}}. \quad (19)$$

Then the Lorentzian focal point  $\mu_{\mathcal{F}}$  can be approximately given as:

$$\mu_{\mathcal{F}} = \sqrt{K} \frac{\sum_{i=1}^m \omega_i x_i}{\|\sum_{i=1}^m \omega_i x_i\|_{\mathcal{L}}}, \quad (20)$$

where  $\omega_i \geq 0$  follows Eq. (18).

#### 4.4 Kernel Mean

The kernel mean [62] can be generalized in Euclidean and hyperbolic geometry, which presents a kernel expression for the geometric mean with respect to the probability measures of Fréchet mean.

We first review some properties of reproducing kernel Hilbert space (RKHS). Let  $\mathcal{H}$  denote a RKHS over  $\mathcal{X}$ , then every bounded linear functional is given by the inner product with a unique vector in  $\mathcal{H}$ . For any  $x \in \mathcal{X}$ , there exists a unique vector  $k_x \in \mathcal{H}$  such that  $f(x) = \langle f, k_x \rangle$  for every  $f \in \mathcal{H}$ . The function  $k_x = K(x, \cdot)$  is called the *reproducing kernel* for point  $x$ , where  $K(x_1, x_2) : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  is positive definite. For any  $k_x, k_y$  in  $\mathcal{H}$ , the Hilbert distance is given as [53]:

$$d_{\mathcal{H}}(k_x, k_y) = \|k_x - k_y\| = \sqrt{\langle k_x - k_y, k_x - k_y \rangle}. \quad (21)$$

Then  $(\mathcal{H}, d_{\mathcal{H}})$  is a complete distance space. Following Eq. (7), Proposition 5 gives a formal description of kernel mean [62].

**Proposition 5.** *Given a separable RKHS  $\mathcal{H}$  endowed with a measurable reproducing kernel  $K(x_1, x_2) : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  such that  $\int d_{\mathcal{H}}^2(k_x, k_y) d\mathbb{P}(x) < \infty$  for all  $y \in \mathcal{X}$ , where  $\mathbb{P}$  denotes a probability measure on  $\mathcal{X}$ . Then the kernel mean  $\mu_{\mathcal{H}}$  minimizes the following problem:*

$$\min_{\mu \in \mathcal{H}} \int d_{\mathcal{H}}^2(k_x, \mu) d\mathbb{P}(x). \quad (22)$$

Based on the completeness of the distance space  $(\mathcal{H}, d_{\mathcal{H}})$ , the following theorem gives the solution of kernel mean, which is consistent with the classical kernel mean defined in [62].

**Theorem 3.** *The kernel mean  $\mu_{\mathcal{H}}$  is unique with the closed-form solution:*

$$\mu_{\mathcal{H}} = \int K(x, \cdot) d\mathbb{P}(x), \quad (23)$$

where  $K(x, \cdot)$  indicates that the kernel has one argument fixed at  $x$  and the second free.

Theorem 3 includes kernel mean in Fréchet mean for the first time, thus maintaining formal uniformity with other standard means, e.g. Euclidean mean. More details and proofs are presented in Appendix.Part B.

## 5 OPTIMIZATION SOLVERS

In order to explore the optimization solvers for the above geometric representations of Euclidean and non-Euclidean paradigms, we category these solvers into three gradient-based methods: Euclidean gradient for the optimization of Euclidean geometric paradigms, Riemannian gradient for optimization of hyperbolic geometric paradigms and Stein gradient for optimization of both Euclidean and hyperbolic geometric paradigms, the details of which are presented as follows.

### 5.1 Euclidean Gradients

**Stochastic Gradient Descent (SGD).** SGD [63] is an effective approach to find the local minima of a cost function, it can be adopted to optimize Euclidean centroids which are formulated as an argmin problem in Euclidean space.

**Stochastic gradient descent.** Given a minimization problem of

$\min_{x \in \mathbb{R}^n} J(x)$  in Euclidean space, at  $t$ -time, the parameters  $x_t$  is updated as [63]:

$$x_{t+1} = x_t - \eta \cdot \nabla_x J(x), \quad (24)$$

where  $J(x)$  denotes the cost function parameterized by  $x$ , and  $\eta$  denotes the learning rate.

### 5.2 Non-Euclidean Gradients

Manifold optimization [64] aims to seek solutions for various constrained optimization problems in Euclidean space by transforming these problems into unconstrained optimization problems on Riemannian manifolds. Correspondingly, Riemannian Gradient Descent (RGD) [65], [66] is introduced to perform iterative optimization. With the scheme, Riemannian optimization domain reaps rapid development. Not surprisingly, hyperbolic geometry also adopt RGD to optimize different paradigms on Poincaré ball  $\mathcal{P}^n$  and Lorentz model  $\mathcal{L}^n$ .

**Riemannian gradient descent.** Given a minimization problem of  $\min_{x \in \mathcal{M}} J(x)$  on a Riemannian manifold  $\mathcal{M}$ ,  $x_t$  at  $t$ -time is updated by the exponential map  $\exp_x$  [66]:

$$x_{t+1} = \exp_{x_t} \left( -\eta J'(x_t) \right), \quad (25)$$

where  $J'(x_t)$  denotes the Riemannian gradient on the tangent space  $T_{x_t} \mathcal{M}$  and  $\eta$  denotes the learning rate.

**Exponential map on Poincaré model.** Given a Riemannian metric  $g_x(\cdot, \cdot)$  that induces an inner product  $\langle u, v \rangle := g_x(u, v)$  on tangent space  $T_x \mathcal{M}$ . For each point  $x \in \mathcal{M}$  and vector  $u \in T_x \mathcal{M}$ , there exists a unique geodesic  $\gamma : [0, 1] \rightarrow \mathcal{M}$  where  $\gamma(0) = x, \gamma' = u$ . The exponential map  $\exp_x : T_x \mathcal{M} \rightarrow \mathcal{M}$  is defined as  $\exp_x(u) = \gamma(1)$ , where  $d_{\mathcal{P}}(x, \exp_x(u)) = \sqrt{g_{\mathcal{M}}(u, u)}$ . With [51],

$$\exp_x(u) = \frac{(1 - 2\langle x, z \rangle_2 - \|z\|^2)x + (1 + \|x\|^2)z}{1 - 2\langle x, z \rangle_2 + \|x\|^2\|z\|^2}, \quad (26)$$

where  $z = \tanh\left(\frac{\|u\|^2}{1 + \|x\|^2}\right) \frac{u}{\|u\|}$ .

**Exponential map on Lorentz model.** With Proposition 3.2 of [57],  $\exp_x(u) = \gamma(1)$  on a Lorentz model  $\mathcal{L}^n$  is expressed as

$$\exp_x(u) = \cosh(\|u\|_{\mathcal{L}})x + u \frac{\sinh(\|u\|_{\mathcal{L}})}{\|u\|_{\mathcal{L}}}. \quad (27)$$

### 5.3 Stein Gradient

Bayesian inference [67] is a statistical inference that invokes the Bayes theorem to approximate the probability distribution. Variational inference [68] approximates parameterized distribution through probabilistic optimization that involves sampling tractable variables, such as Markov Chain Monte-Carlo (MCMC). However, the approximation errors of bayesian and variational inference on estimation over likelihoods or posterior parameter distribution are not easy to control, resulting in unstatistically significant results with calibration. To tight the approximation, Liu *et al.* [69] adopt the Stein operation which controls the bounds on the distance between two probability distributions in a given probability metric. With such proposal, Liu *et al.* then propose the Stein Variational Gradient Descent (SVGD) algorithm [70] that minimizes the KL divergence [71] of two probability distributions  $p$  and  $q$  by utilizing Kernelized Stein Discrepancy (KSD) and smooth transforms, thus conducting iterative probability distribution approximation.

In detail, MCMC estimates the denominator integral of posterior distribution by sampling, thus bringing the problem of computational inefficiencies. Let  $p_0(x)$  be the prior,  $\{D_k\}$  be a set of i.i.d. observations, and  $\Omega = \{q(x)\}$  be the distribution set, variational inference adopts a novel idea to alleviate this by minimizing the KL Divergence between the target posterior distribution  $p(x)$  and another distribution  $q^*(x)$  so as to approximate  $p(x)$ :

$$q^*(x) = \arg \min_{q(x) \in \Omega} \{\text{KL}(q(x)||p(x)) \equiv \mathcal{W}\}, \quad (28)$$

where  $\bar{p}(x) := p_0(x) \prod_{i=1}^N p(D_i|x)$ ,  $Z = \int \bar{p}(x) dx$  denotes the normalization constant which requires complex calculations,  $\mathcal{W} = \mathbb{E}_q[\log q(x)] - \mathbb{E}_q[\log \bar{p}(x)] + \log Z$ . Hence, to circumvent the computation of troublesome normalization constant  $Z$  and seek for a general purpose bayesian inference algorithm, Liu *et al.* adopt the Stein methods and propose the SVGD algorithm. More details are presented in Appendix.Part C.

Given notions of Stein's Identity (Eq. (69)), Stein Discrepancy (Eq. (71)) and Kernelized Stein Discrepancy (Eq. (72)) of the Stein methods, Liu *et al.* rethink the goal of variational inference which is defined in Eq. (28), they consider the distribution set  $\Omega$  could be obtained by smooth transforms from a tractable reference distribution  $q_0(x)$  where  $\Omega$  denotes the set of distributions of random variables which takes the form  $r = T(x)$  with density:

$$q_{[T]}(r) = q(\mathcal{R}) \cdot |\det(\nabla_r \mathcal{R})|, \quad (29)$$

where  $T : \mathcal{X} \rightarrow \mathcal{X}$  denotes a smooth transform,  $\mathcal{R} = T^{-1}(r)$  denotes the inverse map of  $T(r)$  and  $\nabla_r \mathcal{R}$  denotes the Jacobian matrix of  $\mathcal{R}$ . With the density, there should exist some restrictions for  $T$  to ensure the variational optimization in Eq. (28) feasible. For instance,  $T$  must be a one-to-one transform, its corresponding Jacobian matrix should not be computationally intractable. Also, with [72], it is hard to screen out the optimal parameters for  $T$ .

Therefore, to bypass the above restrictions and minimize the KL divergence in Eq. (28), an incremental transform  $T(x) = x + \varepsilon \varphi(x)$  is proposed, where  $\varphi(x)$  denotes the smooth function controlling the perturbation direction and  $\varepsilon$  denotes the perturbation magnitude. With the knowledge of Theorem 5 and Lemma 2, how can we approximate the target distribution  $p$  from an initial reference distribution  $q_0$  in finite transforms with  $T(x)$ ? Let  $s$  denote the total distribution number, an iterative procedure which can obtain a path of distributions  $\{q_t\}_{t=1}^s$  via Eq. (30) is adopted to answer this question:

$$\begin{aligned} q_{t+1} &= q_t[T_t^*], \\ T_t^*(x) &= x + \varepsilon_t \varphi_{q_t, p}^*(x), \end{aligned} \quad (30)$$

where  $T_t^*$  denotes the transform direction at iteration  $t$ , which then decreases the KL Divergence with  $\varepsilon_t \text{KSD}(q_t, p)$  at  $t$ -th iteration. Then, the distribution  $q_t$  finally converges into the target distribution  $p$ . To perform above iterative procedure, Stein Variational Gradient Descent (SVGD) adopts the iterative update procedure for particles which is presented in Theorem 4 to approximate  $\varphi_{q_t, p}^*$  in Eq. (79).

**Theorem 4.** Let  $p(x)$  denote the target distribution,  $\{x_i^0\}_{i=1}^m$  denote the initial particles. Also, at iteration  $t$ , let  $\vartheta = \nabla_{x_j^t} \log p(x_j^t)$ ,  $\mu(x_j^t, x) = \nabla_{x_j^t} k(x_j^t, x)$  denote a regular term,  $\Phi$  denote  $\varepsilon_t \hat{\varphi}^*(x)$ , the particles set are updated iteratively with  $T_t^*$  defined in Eq. (30), in which the expectation under  $q_t$  in  $\varphi_{q_t, p}^*$

is approximated by the empirical mean of  $\{x_i^t\}_{i=1}^m$ :

$$x_i^t + \Phi \rightarrow x_i^{t+1}, \quad (31)$$

where

$$\hat{\varphi}^*(x) = \frac{1}{m} \sum_{j=1}^m [k(x_j^t, x) \vartheta + \mu(x_j^t, x)]. \quad (32)$$

Regarding  $\hat{\varphi}^*(x)$ , the first term  $k(x_j^t, x) \vartheta$  denotes the weighted sum of the gradients of all the points weighted by the kernel function, which follows a smooth gradient direction to drive the particles towards the probability areas of  $p(x)$ ; The second term  $\mu(x_j^t, x)$  denotes a regular term to prevent the collapse of points into local modes of  $p(x)$ , *i.e.*, pushing  $x$  away from  $x_j^t$ .

## 6 LEARNING ON SMALL DATA REPRESENTATION

With the increasing demand of learning on small data, we explore to facilitate the model learning on the small data representation under different future directions, which include Transfer Learning, Meta Learning, Reinforcement Learning, Contrastive Learning, and Graph Representation Learning, *etc.* In this section, we introduce these learning topics and explain the potentiality of learning on small data.

### 6.1 Transfer Learning on Small data

Most of machine learning theories are based on a common assumption: the training and testing data follow the same distribution. However, this assumption is too strict to satisfy or may not hold in many real-world scenarios. Transfer learning [116] loosens the constraint of this assumption (*i.e.*, the training and testing data could be drawn from different distributions or domains), it aims to mining domain-invariant features and structures between different domains so as to conduct effective data and knowledge transfer. Specifically, transfer learning tries to improve the capability of model in target domain by leveraging the knowledge learned from source domain, *e.g.*, transferring the knowledge of riding a bike to driving a car.

One of the core problems of transfer learning according to [116] is that: *What cross-domain knowledge can be migrated to improve the performance of models in target domains?* Although existing solutions can answer this question efficiently in some specific scenarios, there is few general data-driven solutions. Yet, learning on small data provides an appreciable paradigm from the perspective of data representation for crossing-domain knowledge exploitation in transfer learning. Moreover, transfer learning under big data scenarios is inefficient and computational expensive, while learning on small data may alleviate this issue and help harvest more efficient and robust models for its powerful representation capability. Besides, there may exist noisy or perturbed data to be transferred from source domains, which may degenerate the performance of models in target domains, learning on small data may help eliminate such untrustworthy data in transfer learning, thus enhancing the performance of target model. Specifically, we start from the formal definition of transfer learning [116]:

**Definition 7.** *Transfer Learning.* Let  $D_s$  denote a source domain with learning task  $T_s$ ,  $D_t$  denote a target domain and its corresponding learning task is denoted by  $T_t$ . Transfer learning intends to improve the learning performance of the target predictive function  $f_t$  in  $D_t$  with the knowledge learned from  $D_s$  and  $T_s$ , where  $D_s \neq D_t$ , or  $T_s \neq T_t$ .

Table 1: Summary of typical transfer learning strategies

Transfer learning strategies	Main idea
Instance-based strategy	Instances from source domain can be repurposed in target domain by re-weighting [73], [74], [75], [76], [77]
Feature-representation-based strategy	The transferred data across domains is encoded into learned feature representation which can narrow the domain gaps [78], [79], [80], [81], [82], [83], [84]
Parameter-based strategy	The transferred data is encoded into shared parameters or priors between source and target domains [85], [86]
Relational-knowledge-based strategy	Extracting relational-knowledge from different domains to help model learning [87], [88], [89] [90], [91], [92], [93]

Table 2: Summary of typical deep transfer learning strategies

Deep transfer learning strategies	Main idea
Instance-based strategy	Instances from source domain can be repurposed in target domain by re-weighting [94], [95], [96], [97]
Mapping-based strategy	Mapping instances from different domains into a common latent space with small domain gap [98], [99], [100], [101], [102], [103], [104], [105], [106], [107]
Network-based strategy	Reuse the network pre-trained in source domain to help the model learning on target domain [108], [109], [110], [111]
Adversarial-based strategy	Extract transferable knowledge with adversarial-based methods [112], [113], [114], [115]

Based on different situations between the source and target domains and tasks, existing transfer learning methods can be roughly categorized into three settings: inductive transfer learning, transductive transfer learning, and unsupervised transfer learning.

- In **inductive transfer learning**, 1) certain labeled data is available in the target domain with the goal of inducing a predictive model, regardless of whether labeled data is accessible or unavailable in the source domain; 2) the source and target tasks are distinct, but there is no such constraint between the source and target domains.
- In **transductive transfer learning**, 1) there is a lot of labeled data available in the source domain while the target domain lacks any labeled data; 2) the source and target tasks are same, but the source and target domains are different.
- In **unsupervised transfer learning**, 1) there is no labeled data available in both source and target domains, except for the unsupervised tasks of target domain; 2) the target and source tasks are distinct but related, while the source and target domains have no such constraint.

On the above three settings, Table 1 summarizes the popular strategies of transfer learning based on the type of data to be transferred. Furthermore, deep learning has been widely explored in transfer learning to leverage the knowledge obtained from source domains for deep neural networks. Formally, deep transfer learning [117] is defined as follows.

**Definition 8. Deep Transfer Learning.** Let  $T_s$  be a deep learning task in source domain  $D_s$ ,  $T_t$  be a deep learning task in target domain  $D_t$ , deep transfer learning is to improve the performance of a deep neural network with a non-linear target predictive function  $f_t$  in  $D_t$  by extracting knowledge from  $D_s$  and  $T_s$ , where  $D_s \neq D_t$ , or  $T_s \neq T_t$ .

Similar to non-deep transfer learning strategies, deep transfer learning strategies can also be classified into four categories [117] which are summarized in Table 2. It is full of potential to introduce learning on small data to transfer learning [118]. For instance, in

non-deep transfer learning, the significant and informative small data obtained from source domain could be utilized to perform instance transfer by re-weighting [74]; By analogy, in deep transfer learning, we can also conduct instance transfer with the small data by deep neural networks as well. Moreover, in different scenarios of feature-representation transfer learning, the domain-invariant features may also be efficiently extracted with small data learning methods [83], [119], [84]. Similarly, in the context of deep transfer learning, extracting partial instances in the source domain of instance-based deep transfer learning, reusing partial network which is pre-trained in the source domain of network-based deep transfer learning and extracting transferable representations [120] applicable to both the source domain and the target domain in deep transfer learning can reap better performance with the power of learning on small data. In conclusion, learning on small data could be adopted to various transfer learning scenarios, it still awaits in-depth research.

## 6.2 Meta-learning on Small data

Conventional machine learning models are typically trained on a dataset exclusive to a given task, thus resulting in a problem of poor generalization, that is, it is difficult for the learning models to adapt to previously unseen tasks. To relieve this difficulty, meta-learning [121] utilizes the well-generalized meta-knowledge, e.g. the tuned learning parameters across various learning tasks, to teach the *learning models* to learn for unseen tasks.

Therefore, how to extract well-generalized meta-knowledge [122] has become an critical issue in meta-learning. Moreover, there may exist few efficient data and labels in many meta-learning scenarios, so it is of great importance to explore how to extract efficient data or improve the performance of models with small data. Learning on small data has been trying for this, it may provide novel ideas to obtain meta-knowledge which can help alleviate overfitting and enhance the generalization capability for the model. Furthermore, during the meta-training phase, learning on small data may contribute to the selection of representative and impactful meta-tasks so as to harvest a robust meta-learning model. Specifically, We then start from a comprehensive overview

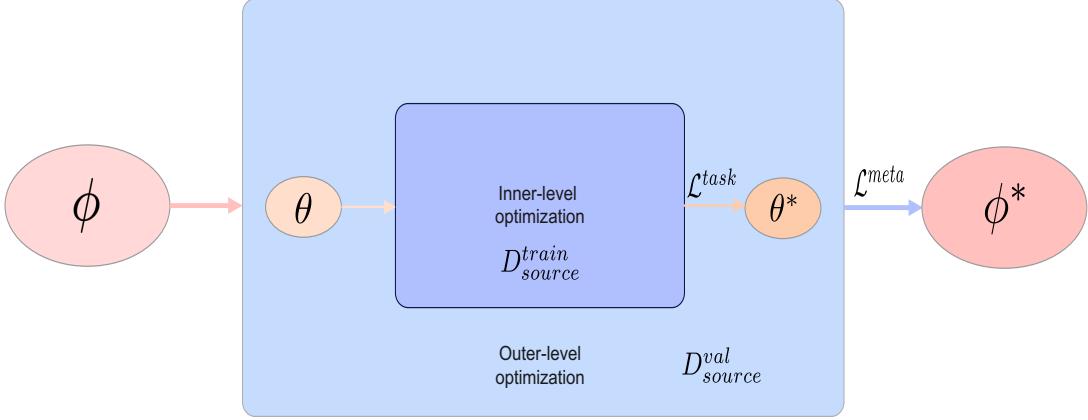


Figure 2: The bilevel optimization perspective of meta-learning. During the meta-training phrase, the inner-level optimization is to train the model on different tasks which are sampled from  $D_{source}^{train}$  to obtain the optimal model with parameters  $\theta^*$ ,  $\mathcal{L}^{task}$  denotes the optimization objective for inner-level optimization; the outer-level optimization aims to obtain a general meta-knowledge  $\phi^*$  which be quickly adapted to unseen tasks.  $\mathcal{L}^{meta}$  denotes the optimization objective to obtain  $\phi^*$ .

of meta-learning from three different perspectives [121].

**Task-Distribution Perspective.** From the perspective of task-distribution [123], [124], meta-learning considers tasks as samples of the model. Besides, this learning paradigm aims to learn a common learning algorithm which can generalize across tasks. In detail, the goal of meta-learning is to learn a general meta-knowledge  $\phi$  which can minimize the expected loss of meta-tasks. Let  $q(\mathcal{T})$  denote the distribution of tasks,  $D$  denote the dataset for meta-tasks, meta-learning can be formalized as:

$$\min_{\phi} \mathbb{E}_{\mathcal{T} \sim q(\mathcal{T})} \mathcal{L}(D; \phi), \quad (33)$$

where  $\mathcal{L}(D; \phi)$  denotes the loss function to measure the performance of meta-learning model. To address the optimization problem, it is assumed that we can obtain a set of source tasks sampled from  $q(\mathcal{T})$ . With [121], meta-learning consists of two phases: **meta-training** phrase and **meta-testing** phrase. Let  $\mathcal{D}_{source} = \{(D_{source}^{train}, D_{source}^{val})^{(i)}\}_{i=1}^M$  denote the set of  $M$  source tasks in meta-training phase, where  $D_{source}^{train}$  and  $D_{source}^{val}$  denote the training and validation data respectively for source tasks, the serial number  $i$  indicates each task;  $\mathcal{D}_{target} = \{(D_{target}^{train}, D_{target}^{test})^{(i)}\}_{i=1}^N$  denote the set of  $N$  target tasks in meta-testing phase, where  $D_{target}^{train}$  and  $D_{target}^{test}$  denote the training and testing data for target tasks, respectively. On this setting, the meta-training phrase is to learn the optimal meta-knowledge  $\phi^*$  and maximize the log likelihood by sampling different source tasks from  $\mathcal{D}_{source}$ , it is thus formalized as:

$$\max_{\phi} \log p(\phi | \mathcal{D}_{source}). \quad (34)$$

By solving such a maximum problem, we obtain a well-generalized meta-knowledge  $\phi^*$ , which is utilized to facilitate the model learning on unseen target tasks. The meta-testing phase aims to obtain a robust model on the training data of each unseen target task sampled from  $\mathcal{D}_{target}$  with the help of  $\phi^*$ , which can be formalized as:

$$\max_{\theta} \log p(\theta | \phi^*, D_{target}^{train}). \quad (35)$$

We can thus obtain a model with parameters  $\theta^*$  by solving the above maximum problem and evaluate its performance by conduct

target tasks which are sampled from  $D_{target}^{test}$ .

**Bilevel Optimization Perspective.** Bilevel optimization [125], [126], [127] is a hierarchical optimization problem, which means one optimization objective contains another inner optimization objective as a constraint. Therefore, from the perspective of bilevel optimization [128], [129], the meta-training phrase is formalized as:

$$\begin{aligned} \phi^* &= \arg \min_{\phi} \sum_{i=1}^M \mathcal{L}^{meta} \left( \theta^{*(i)}(\phi), \phi, D_{source}^{val(i)} \right) \\ \text{s.t. } \theta^{*(i)}(\phi) &= \arg \min_{\theta} \mathcal{L}^{task} \left( \theta, \phi, D_{source}^{train(i)} \right), \end{aligned} \quad (36)$$

where  $\mathcal{L}^{meta}$  and  $\mathcal{L}^{task}$  denote the outer and the inner loss objectives, respectively. The inner-level optimization is with  $\phi$  which is defined in outer-level optimization as condition, but  $\phi$  cannot be changed during the inner-level optimization phrase; the outer-level optimization utilize  $\theta^{*(i)}(\phi)$  obtained from the inner-level optimization to optimize the meta-knowledge  $\phi$ . The bilevel optimization scheme of meta-learning is presented in Figure 2.

**Feed-Forward Perspective.** With [121], there exists different meta-learning methods which synthesize models in feed-forward manners [131], [132]. Let  $\gamma = \mathbf{x}^\top \mathbf{e}_\phi(D^{train})$ , a simple example for meta-training linear regression objective which optimizes over a distribution of meta-training tasks from feed-forward perspective is defined as:

$$\min_{\phi} \mathbb{E}_{\mathcal{T} \sim q(\mathcal{T})} \sum_{(\mathbf{x}, y) \in \mathcal{D}^{val}} [(\gamma - y)^2], \quad (37)$$

where the training set  $\mathcal{D}^{train}$  is embedded into the vector  $\mathbf{e}_\phi$  which defines the linear regression weights, thus making prediction of samples  $\mathbf{x}$  from the validation set  $\mathcal{D}^{val}$ .

With the above three perspectives, we can also introduce learning on small data to different meta-learning scenarios for the reason that meta-learning can utilize the knowledge obtained by small data learning methods to get with unseen tasks. For example, meta-learning cares about the choice of meta-knowledge  $\phi$ , it is potential that learning on small data can assist the selection of  $\phi$  such as assigning different impact factors to inner-level tasks [133], [134] so as to influence the final gradient direction during

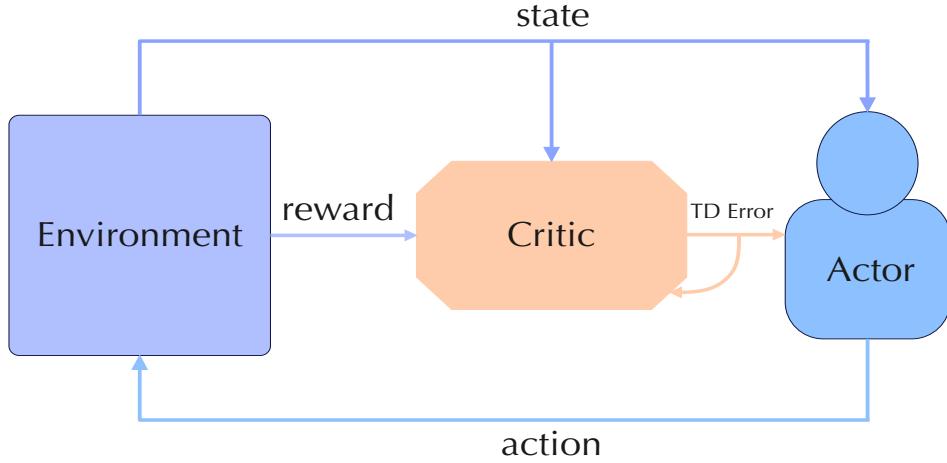


Figure 3: The illustration of actor-critic strategies in reinforcement learning. There are three objects in the scheme: Environment, Critic (value function) and Actor (policy). Environment interacts with Critic and Actor by providing rewards to Critic, states to both Critic and Actor. Then, Actor conducts an action refer to the provided state, meanwhile, Critic learns about and criticizes the action conducted by Actor. TD Error is introduced to evaluate the critique process and drives the updates of both Critic and Actor. Recreated from [130].

the process of inner-level optimization. Moreover, task sampling performs an indispensable role for meta-learning model, learning on small data may help sample significant meta-tasks during meta-training phrase: from bilevel optimization perspective, small data learning methods can be adopted to guide task sampling of inner-level optimization to obtain a better  $\theta^*$ , which may ultimately enhance the performance of meta-learning model. Besides, with [121], learning on small data can be introduced to different applications of meta-learning such as parameter initialization, embedding functions, modular meta-learning. Therefore, it is promising to introduce learning on small data to meta-learning.

### 6.3 Reinforcement Learning on Small data

Reinforcement learning [135] is an AI paradigm which emphasizes on maximizing the desired benefits by rewarding expected actions and/or punishing unexpected ones. In reinforcement learning, there are two interactive objects: *Agent* and *Environment*. *Agent* can perceive the state of *Environment* and reward the feed-backs from *Environment*, thus making sound decisions. In other words, the decision-making function of *Agent* takes different actions according to the state of *Environment*, while learning function adjusts policies according to the rewards from *Environment* which can adjust its states under the influence of *Agent*'s action and feed back to *Agent* the corresponding rewards.

Yet, with [136], reinforcement learning still confronts with many challenges, one of which is: learning on the real system from limited samples. Besides, deep reinforcement learning strategies require active online data collection which means it may be expensive to collect large-scale data during such process. Learning on small data may help extract valuable prior knowledge from previously collected interaction data, it enables us to pre-train and deploy *Agents* capable of learning efficiently. In addition, efficient data extracted by learning on small data contributes to the model obtaining better generalization performance. Therefore, learning on small data could be considered as a novel data-driven paradigm for reinforcement learning.

Specifically, reinforcement learning strategies could be categorized into value-based, policy-based and actor-critic strategies

[130].

**Value-based strategies.** Value-based strategies [137], [138] are introduced for estimating the expected under a specified state. The state-value function  $V_\pi(s)$  which denotes the expected return given state  $s$  and policy  $\pi$  is formalized as:

$$V_\pi(s) = \mathbb{E}[\mathcal{R}|s, \pi]. \quad (38)$$

Since  $V_\pi(s)$  is designed for evaluating policy  $\pi$ , all polices can be evaluated to obtain the optimal policy  $\pi^*$  and the corresponding state-value function  $V_{\pi^*}(s)$  is defined as:

$$V_{\pi^*}(s) = \max_\pi V_\pi(s), \quad \forall s \in S, \quad (39)$$

where  $S$  denotes the state set. Hence, we can obtain  $\pi^*$  by greedy search among all actions at  $s_t$  and taking the action  $a$  which maximizes the following objective:

$$O = \mathbb{E}_{s_{t+1} \sim \mathcal{T}(s_{t+1}|s_t, a)} [V_{\pi^*}(s_{t+1})], \quad (40)$$

where  $\mathcal{T}(s_{t+1}|s_t, a)$  is the so-called *transition dynamics* which construct a mapping of state-action pair at time  $t$  onto a set of states at time  $t + 1$ . However, with [130], it is common sense that  $\mathcal{T}$  is not available in RL settings. Therefore, the so-called *Q-function*:  $Q_\pi(s, a)$  is introduced as the alternative to  $V_\pi(s)$ :

$$Q_\pi(s, a) = \mathbb{E}[\mathcal{R}|s, a, \pi], \quad (41)$$

where the initial action  $a$  and the following policy  $\pi$  is pre-given.  $Q_\pi(s, a)$  denotes the expected return value of taking an action  $a$  in a state  $s$  following the policy  $\pi$ . Thus, given  $Q_\pi(s, a)$ , the optimal policy  $\pi^*$  can be obtained by the greedy search among all actions and the corresponding  $V_{\pi^*}(s)$  can be defined as:

$$V_{\pi^*}(s) = \max_a Q_\pi(s, a). \quad (42)$$

Therefore, it is vital to learn  $Q_\pi$  in such a scheme. Let  $\mathcal{H}$  denote  $Q_\pi(s_{t+1}, \pi(s_{t+1}))$ , and the recursive form of  $Q_\pi$  can be obtained by utilizing the notion of Markov property and Bellman equation [139]:

$$Q_\pi(s_t, a_t) = \mathbb{E}_{s_{t+1}} [r_{t+1} + \gamma \mathcal{H}], \quad (43)$$

where  $r_{t+1}$  denotes the immediate rewards at time  $t + 1$ ,  $\gamma \in [0, 1]$  denotes the discount factor for moderating the weight of short-term rewards and long-term rewards. When  $\gamma$  is close to 0, *Agent* cares more about short-term rewards; On the contrary, when  $\gamma$  is close to 1, *Agent* cares more about long-term rewards.

**Policy-based strategies.** Different from value-based strategies, policy-based strategies [140], [141], [142], [143], [144] do not depend on a value function, but greedily search for the optimal policy  $\pi^*$  in the policy space. Most policy search strategies perform optimization locally around all policies which are parameterized by a set of policy parameters  $\eta_i$  respectively. The update of the policy parameters adopts a gradient-based way which follows the gradient of the expected return  $E$  with a pre-defined step-size  $\alpha$ :

$$\eta_{i+1} = \eta_i + \alpha \nabla_\eta E. \quad (44)$$

There exists various approaches to estimate the gradient  $\nabla_\eta E$ . For instance, in finite difference gradients, the estimate of the gradient can be obtained by evaluating  $G$  perturbed policy parameters. Given  $\Delta E_g \approx E(\eta_i + \Delta \eta_g) - E_{ref}$ , where  $g = [1, 2, \dots, G]$  denotes the perturbations,  $\Delta E_g$  denotes the estimate of influence of  $g$  on the expected return  $E$  and  $E_{ref}$  denotes a reference return (e.g., the return of the unperturbed parameters), let  $L = \Delta \Upsilon^\top \Delta \Upsilon$ ,  $\nabla_\eta E$  can thus be estimated by

$$\nabla_\eta E \approx L^{-1} \Delta \Upsilon^\top \Delta \tilde{E}, \quad (45)$$

where  $\Delta \Upsilon$  denotes a matrix which contains all the samples of the perturbations  $\Delta \eta_g$  and  $\Delta \tilde{E}$  denotes the matrix contains the corresponding  $\Delta E_g$ .

**Actor-critic strategies.** Actor-critic strategies [145], [146], [147], [148], [149], [150], [151] aim to combine the benefits of both policy search strategies and learned value functions. Here “actor” denotes the policy  $\pi$ , “critic” denotes the value function. The “actor” learns by the feedback from the “critic”, which means actor-critic strategies can obtain effective policies by continuous learning so as to achieve high returns. Different from common policy gradient strategies which utilizes the average of several Monte Carlo returns as the baseline, actor-critic strategies can learn from full returns and TD errors. Once policy gradient strategies or value function strategies make progress, actor-critic strategies may also be improved. The detailed illustration of actor-critic strategies is presented in Figure 3.

Learning on small data may also effectively perform its role and demonstrate great potential for reinforcement learning. For instance, small data learning methods can be adopted to value-based strategies while evaluating all policies by influencing the expected return to obtain the optimal policy  $\pi^*$  [137]. Moreover, during the process of direct policy search for the optimal policy in policy-based strategies, small data learning methods can effectively act as the auxiliary role such as perturbing the direction of policy gradient, thus influencing the final decision of policy search. Besides, in actor-critic strategies, small data learning methods can assist in the adjustment of scores from the “critic” [152]. In conclusion, learning on small data may act as an important assisting role in various reinforcement learning scenarios to enhance the generalization performance and robustness of models, it still awaits in-depth exploration for the integration of the two fields.

#### 6.4 Contrastive Learning on Small data

Self-supervised learning [153] has obtained interests thanks to its capacity to avoid the cost of annotating large-scale datasets.

It mainly utilizes pretext tasks to mining the supervision information from unsupervised data. With the constructed supervision information, we may conduct the model learning and obtain valuable representations for downstream tasks. Meanwhile, contrastive learning [154], [155], [156], [157], [158] has recently become a significant sub-topic in self-supervised learning, it aims to learn a representation which can group positive pairs closer and push away negative pairs in the latent embedding space with contrastive loss. A learning step in contrastive learning is presented in Figure 4.

Wu *et al.* [159] put that contrastive learning usually generates multiple views for each data instance via data augmentation methods. Two views generated from the same sample are positive pairs while from different data samples are negative pairs. Maximizing the agreement of two combined positive pairs against the agreement of two independent positive pairs is the ultimate goal and the agreement between views can be measured by Mutual Information (MI) estimation which is given as

$$MI(v_i, v_j) = \mathbb{E}_{p(v_i, v_j)} \left[ \log \frac{p(v_i, v_j)}{p(v_i)p(v_j)} \right], \quad (46)$$

where  $v_i$  and  $v_j$  denote different views,  $p(v_i, v_j)$  denotes the joint distribution of  $v_i$  and  $v_j$ . Besides,  $p(v_i)$  and  $p(v_j)$  denote the marginal distributions of  $v_i$  and  $v_j$  respectively.

Although contrastive learning makes great efforts to learn a valuable representation, there may often exist few efficient data in various contrastive learning scenarios, thus setting restrictions on achieving the goal. Learning on small data takes full account of the cases, it is dedicated to providing efficient and general solutions under small data scenarios. Furthermore, *How to seek representative samples to generate contrastive pairs* [160], [161] is one of the most significant issues in contrastive learning. Besides, appropriate data augmentation strategies in contrastive learning to obtain efficient positive samples can greatly improve the representation capability and generalizability of models. Learning on small data can thus be considered as a novel perspective for the choice of anchor samples and the guidance of data augmentation strategies. In addition, with [162], contrastive learning benefits from hard negative samples. Learning on small data contributes to finding the truly *hard* negative samples so as to improve the performances of contrastive learning models. Through the above perspectives, learning on small data deserves further exploration to promote the development of contrastive learning.

Learning on small data may perform an effective role for view selection in contrastive learning [156], *i.e.*, the choice of positive pairs (by data augmentation methods) or negative pairs (by negative sampling methods). More specifically, the representative samples chosen by small data learning methods can be considered as the anchors, thus we can obtain the augmented versions of them with various data augmentation methods. Under the scheme, the augmented version of the anchors could be considered as positive samples and the rest of the training data are viewed as negative samples. Furthermore, learning on small data may help extract truly *hard* negative samples so as to enhance the performance of models [154], it may also help evaluate and design reasonable  $\mathcal{L}_{contrastive}$  to reap a robust contrastive learning model. To conclude, learning on small data can be adopted to different sections of the complete pipeline and assist the contrastive learning models to harvest great generalizability and promising performance.

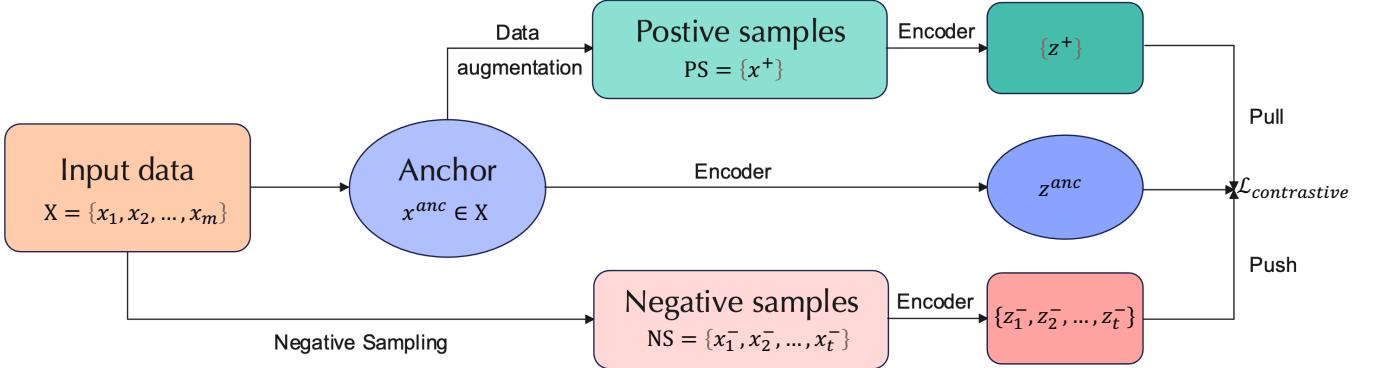


Figure 4: Learning step of contrastive learning. Contrastive learning aims to learn an effective encoder to embed the samples into a latent embedding space, it pulls closer the embedded anchor  $z^{anc}$  and the positive embeddings  $\{z^+\}$ , pushes away  $z^{anc}$  and the negative embeddings  $\{z_1^-, z_2^-, \dots, z_t^-\}$ .  $\mathcal{L}_{contrastive}$  is introduced to evaluate the performance of the learning step.

## 6.5 Graph Representation Learning on Small data

Graph is a common data structure for describing complicated systems such as social networks, recommendation system. Over the past several years, due to the great expressive power of graph, graph representation learning [163] has gradually attracted the attention of machine learning community, it aims to build models which can efficiently learn from non-Euclidean data. Meanwhile, various graph neural networks [164] emerge as the times require, they show great potential in structured-data mining tasks, e.g., node classification, link prediction, or graph classification.

However, when these graph data mining tasks meet many unsupervised / supervised scenarios where few, even no efficient data or labels exist, how to enhance the performances of these tasks on graphs and obtain a robust model in these cases? Meanwhile, there still exists many meaningful sub-topics to be explored such as relationship structure discovery [165], [166], [167], representational power [168] of graph neural networks which may also needs effective ideas from data representation perspective. With regard to the above mentioned issues, learning on small data may provide necessary and powerful support, it may promote the development of graph representation learning due to its appreciable data discovery efficiency and strong representational capability.

In particular, a general design pipeline for GNNs is presented in Figure 5. Under the scheme of this design pipeline, GNNs can be categorized into recurrent graph neural networks, convolutional graph neural networks, graph autoencoders and spatial-temporal graph neural networks. Detailed description of the taxonomy is presented as follows [164].

**Recurrent graph neural networks (RecGNNs).** RecGNNs are designed to learn node representation with recurrent neural networks. In detail, RecGNNs leverage the same recurrent models over nodes to obtain high-level representations [164]. Under the scheme, let  $l_{vq} = x_e(v, q)$  denote the features of edge linking node  $v$  and node  $q$ , the hidden state of node  $v$  at time  $t$  is recurrently updated by

$$h_v^{(t)} = \sum_{q \in N(v)} f(x_v, x_q, l_{vq}, h_v^{(t-1)}), \quad (47)$$

where  $N(v)$  denotes the neighborhood set of node  $v$ ,  $x_v$  and  $x_q$  denote the node features of  $v$  and  $q$  respectively,  $f(\cdot)$  denotes the recurrent function which must be a contraction mapping for

mapping different nodes into the same latent space so as to narrow the distance between the embedded ones. What follows are a series of RecGNNs such as Graph Echo State Network (GraphESN) [164], Gated Graph Neural Network (GGNN) [169] and Stochastic Steady-state Embedding (SSE) [170].

**Convolutional graph neural networks (ConvGNNs).** Learning from traditional convolution operation on grid data, ConvGNNs aim to extract the high-level representations of nodes by graph convolution operation and feature aggregation. Specifically, ConvGNNs approaches could be categorized into spectral-based and spatial-based [171]. Spectral-based approaches adopt graph convolution operation from the perspective of graph signal processing [172] and the spatial-based ones define graph convolutions from the perspective of information propagation [173]. For spectral-based ConvGNNs, let  $l$  denote the layer index,  $g_\theta = \Omega_{i,j}^{(l)}$  denote the convolution filter which is a diagonal matrix composed of learnable parameters,  $c_{l-1}$  denote the number of input channels,  $H^{(l-1)}$  denote the input graph signal, the definition of graph convolutional layer of spectral-based ConvGNNs is given as:

$$H^{(l)} = \sigma \left( \sum_{i=1}^{c_{l-1}} U \Omega^{(l)} U^\top H^{(l-1)} \right), \quad (48)$$

where  $U = [u_0, u_1, \dots, u_{n-1}] \in R^{n \times n}$  denotes the matrix composed of eigenvectors which can be obtained by decomposing the normalized Laplacian matrix. In following works, ChebNet [174] performs approximations of filter  $g_\theta$  with Chebyshev polynomials, GCN [175] introduces a first-order approximation of ChebNet, which reduces the computational complexity. After this, various variants such as AGCN [176], DGCN [177] expand upon GCN.

Neural Network for Graphs (NN4G) [178] is the first one of spatial-based ConvGNNs, it performs graph convolutions by neighborhood information aggregation and leverages residual connections and skip connections to preserve information over each layer. Let  $\Gamma$  denote  $\sum_{i=1}^{l-1} \sum_{q \in N(v)} \Omega^{(l)} h_q^{(l-1)}$ , the hidden state of NN4G is formalized as:

$$h_v^{(l)} = f(W^{(l)} x_v + \Gamma), \quad (49)$$

where  $W^{(l)}$  is the weight matrix composed of learnable parameters,  $\Omega^{(l)}$  denotes the matrix which consists of filter parameters. Let  $\Psi = \sum_{i=1}^{l-1} A \Omega^{(l)} H^{(l-1)}$ , Eq. (49) can also be given in matrix

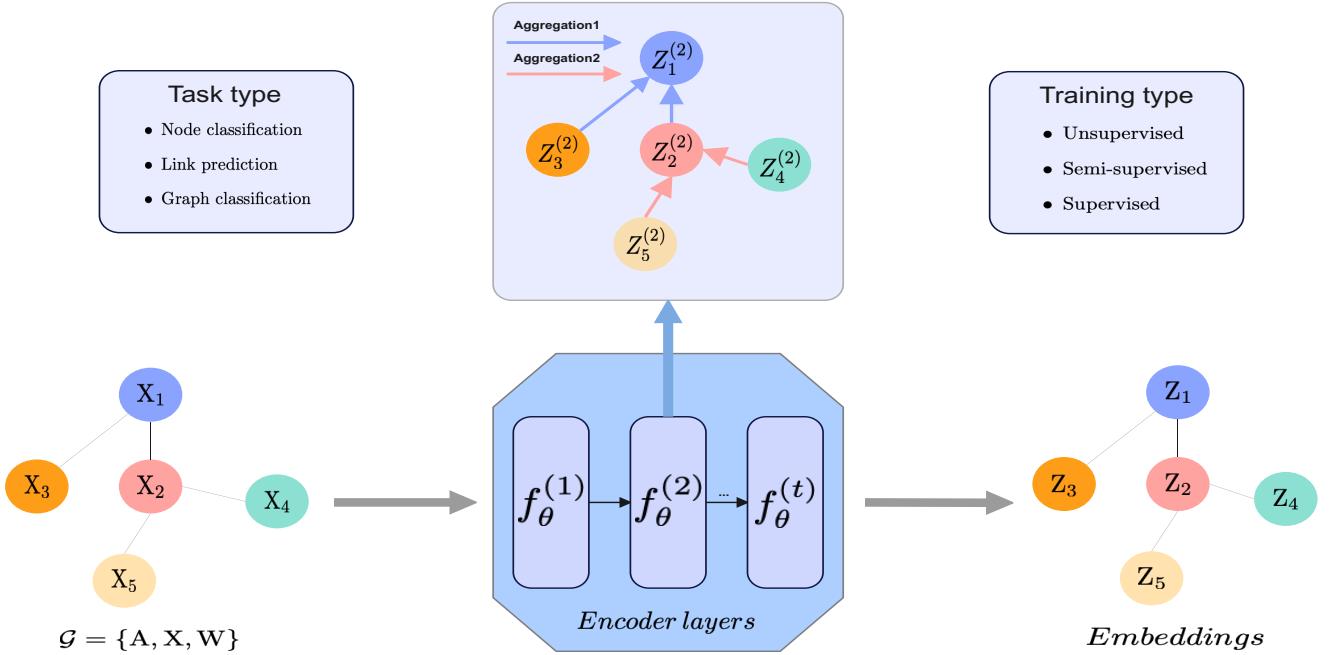


Figure 5: A general design pipeline for GNNs. For an input graph  $\mathcal{G} = \{\mathbf{A}, \mathbf{X}, \mathbf{W}\}$ ,  $\mathbf{A}$  denotes the adjacency matrix of  $\mathcal{G}$ ,  $\mathbf{X}$  denotes the feature matrix of all nodes in  $\mathcal{G}$ ,  $\mathbf{W}$  denotes the weight matrix composed of learnable parameters which can be dynamically adjusted during training. Multiple encoder layers are introduced to encode  $\mathcal{G}$  into the corresponding embeddings. In each encoder layer, message passing and neighborhood aggregation are conducted.

form:

$$\mathbf{H}^{(l)} = f(\mathbf{W}^{(l)}\mathbf{X} + \Psi), \quad (50)$$

where  $\mathbf{A}$  denotes the adjacency matrix of a graph which indicates connection information between nodes. In addition, Diffusion Convolutional Neural Network (DCNN) [179], Partition Graph Convolution (PGC) [180], Message Passing Neural Network (MPNN) [181], Graph Isomorphism Network (GIN) [182], Graph Attention Network (GAT) [183] and various spatial-based ConvGNNs variants emerge as the times require.

**Graph autoencoders (GAEs).** GAEs encode nodes or graphs into a latent space and decode the corresponding information from the latent representation [184]. In other words, GAEs learn the embeddings with encoder-decoder architecture, where the encoder aims to embed the network into a latent space and the decoder decodes graph information from the embeddings. Following this way, a series of GAE variants burst forth such as Deep Neural Network for Graph Representations (DNGR) [185], Structural Deep Network Embedding (SDNE) [186], Variational Graph Autoencoder (VGAE) [184], Adversarially Regularized Variational Graph Autoencoder (ARVGA) [187], GraphSage [188]. Take GraphSage as an example, let  $\text{dec}(\cdot)$  be a decoder which consists of a multi-layer perceptron,  $\mathbf{z}_v$  and  $\mathbf{z}_q$  denote the embeddings of two nodes in graph,  $Q$  be the number of negative samples,  $D_1 = \text{dec}(\mathbf{z}_v, \mathbf{z}_q)$ ,  $D_2 = -\text{dec}(\mathbf{z}_v, \mathbf{z}_{v_i})$ , GraphSage [188] puts that the negative sampling with the loss below can preserve significant information of nodes such as the relational information between two nodes,

$$L(\mathbf{z}_v) = -\log(D_1) - Q \mathbb{E}_{v_i \sim D_i(v)} \log(D_2), \quad (51)$$

where node  $\mathbf{z}_{v_i}$  denotes a distant node from  $\mathbf{z}_v$  sampled from  $D_i(v)$  which denotes the negative sampling distribution,  $L(\mathbf{z}_v)$

considers that close nodes tend to share similar representations and distant nodes to have dissimilar representations.

**Spatial-temporal graph neural networks (STGNNs).** The goal of STGNNs is to learn hidden patterns from spatial-temporal graphs [189], [190]. In other words, STGNNs take spatial dependencies and temporal dependencies of a graph into account at the same time. With [164], it can be categorized into RNN-based methods and CNN-based methods. RNN-based methods may balance the spatial and temporal dependencies by leveraging graph convolutions to handle the input graph and hidden states committed to a recurrent unit. Let  $G_1 = G\text{conv}(\mathbf{X}^{(t)}, \mathbf{A}; \mathbf{W})$ ,  $G_2 = G\text{conv}(\mathbf{H}^{(t-1)}, \mathbf{A}; \mathbf{U})$ , a simple RNN with graph convolution is given as:

$$\mathbf{H}^{(t)} = \sigma(G_1 + G_2 + b), \quad (52)$$

where  $\mathbf{X}^{(t)}$  denotes the feature matrix of a node at time  $t$ ,  $G\text{conv}(\cdot)$  denotes the graph convolutional layer and  $b$  denotes the bias. Graph Convolutional Recurrent Network (GCRN) [191], Diffusion Convolutional Recurrent Neural Network (DCRNN) [192] and other variants follow this way. However, RNN-based methods require much computational time during the iterative propagation phase. Besides, RNN-based methods suffer from the vanishing / exploding gradient problem [193]. By contrast, CNN-based methods run in a non-recursive manner which means they possess the advantages of parallel computing, stable gradients and low memory requirements. Spatio-temporal Graph Convolutional Networks (CGCN) [194], Spatial-temporal Graph Convolutional Networks (ST-GCN) [195] and a series of other variants follow the paradigm.

Can learning on small data truly benefit graph representation learning? The answer is: exactly. For example, in the context of graph statistical characteristics, node centrality metrics [196] in-

cludes degree centrality, closeness centrality, eigenvector centrality, betweenness centrality, *etc.* It is promising to adopt small data learning methods to explore more centrality metrics to measure the importance of nodes in a graph. Moreover, learning on small data may introduce novel ideas focusing on extracting efficient data for graph representation learning with only few data such as self-supervised learning on graphs. Besides, in some graph neural networks, we can also introduce learning on small data to obtain better neighborhood aggregation or message passing schemes such as defining how important the message from a neighbor is to a node, thus improving the performance of models in downstream tasks. In conclusion, it is full of potential to integrate learning on small data and graph representation learning to explore more possible collaborable scenarios.

## 7 CHALLENGING LEARNING SCENARIOS

In this section, we introduce some challenging but practical learning settings. They become even troublesome in the small data regime, however, new opportunities also arise, which can broaden the applications of the methods for small data.

### 7.1 Deep Learning Scenario

Deep learning is one of the recent trending topics. It significantly pushes forward the state-of-the-art of various tasks [197]. However, deep models are usually data-hungry due to their massive parameters, which lead to unfriendly tuning for applications. To tackle with this challenging problem, many works are proposed to reduce the amount of data for model training. Thus, we summary some related techniques and provide possible future directions for deep learning with small data.

To fully exploit the limited labeled examples, data augmentation [198] is one of the most important techniques to enhance the performance without extra data requirements. It transforms the examples without changing the semantics to help the model learning. With the recent advances of Generative Adversarial Network (GAN) [199], some studies also propose to generate more examples to augment the training set. Another method is to exploit the unlabeled data. One can assign pseudo-labels to the unlabeled data, which can be achieved by, *e.g.*, co-training [200], semi-supervised learning [201]. Alternatively, unsupervised representation learning methods, *e.g.*, contrastive learning [202], can also be employed to enhance the feature extraction. It constructs a pretext task on the unlabeled data for representation learning, then adapt to the downstream tasks. To show the effectiveness of this technique, Chen *et al.* [203] report that they use only 10% of the labels to fine-tune the pre-trained network, and achieve a comparable performance with the model trained with all labels from scratch for 90 epochs in ImageNet ILSVRC-2012 dataset. Active learning [204] and transfer learning have also been widely applied in training deep models. The former selectively queries informative data for labeling, while the latter introduces external knowledge to help the model training (*e.g.*, by domain adaptation [205]). Both of them are well validated to reduce the label requirement of training an effective deep model.

Possible future directions may include the interpretable deep learning methods [206], so that we can incorporate prior knowledge to help the learning on small data. Besides, effective model selection methods with small data may also improve the performances by choosing suitable network architectures.

### 7.2 Weakly-supervised Scenario

Most of machine learning studies assume that the data can be accurately annotated with the ground-truth labels. However, in many real learning scenarios, the supervision can not meet this assumption due to the lack of perfect annotators, which leads to the noisy and inexact labels [207]. The former case includes mislabeled training data, the latter case includes redundant labels, insufficient labels and coarse labels. Such learning scenarios become more tough in the small data regime. To help getting over this obstacle, we review some related methods and provide possible directions for the research on small data under this challenging setting.

**Noisy label.** To tackle with the noisy supervision in small data, possible solutions include noise level control and robust learning methods. The former can be implemented by, for example, active learning to query the easy but informative examples [208] or query from the high quality annotators [209] in order to reduce the noise level with limited budget. Another related technique for the low cost regime may be the active label cleaning [210], which tries to actively rectify the most valuable mislabeled data. We note that identifying the informative noise data will be more challenging with only limited examples. For the latter case, some related explorations, *i.e.*, noisy few-shot learning, are conducted to learn robust representation with small data. For example, Gao *et al.* [211] propose a hybrid attention technique to solve the noisy few-shot relation classification task. They apply the attention modules to the prototypical networks to emphasize the crucial instances and features, so that the influence of the noise can be alleviated. Liang *et al.* [212] propose a feature aggregation method adopted in a transformer architecture to capture those noises by re-weighting images. The experimental results show that their proposed method can achieve better performance in the noisy setting compared to the state-of-the-art few-shot learning approaches.

For the possible future directions, we believe the transfer learning and meta learning may be effective to improve the robustness of the model to the noise based on small data by introducing extra knowledge. Besides, exploiting the unlabeled data (*e.g.*, semi-supervised learning, contrastive learning) may also provide useful information for learning on limited noisy labels.

**Inexact label.** For the inexact labels under small data regime, there are some pioneer works that try to utilize the unlabeled data to improve the representation learning. For example, Xie and Huang [213] tackle with the semi-supervised partial multi-label learning, where each labeled data are annotated with all relevant labels and some redundant labels. They exploit the unlabeled data to learn a low-dimensional embeddings and achieve better performances. Other possible techniques include the graph representation learning, which is well-suited to the inexact supervision setting due to its great potential in label completion [214]. Transfer learning is also a commonly used approach to complement the absent supervision from a related fully-supervised source domain, *e.g.*, Cao *et al.* [215] propose a category transfer framework to help the object detection model training on the images with only class label annotation. It can handle both overlapping and non-overlapping category transfer, thus has wide applications.

Look into the future, we also believe that the unsupervised learning techniques, *e.g.*, contrastive learning, clustering, may help the model training on inexact supervised small data. Alternatively, active learning with inexact label querying may also be a promising direction. Because in some cases, the model may not need

all information of a fully supervised example, thus querying the essential partial supervision can be a more cost-effective choice.

### 7.3 Multi-label Scenario

Multi-label learning [216] studies the setting that each instance is associated with multiple categories, *i.e.*, map the data into  $2^C$  dimensional label space with  $C$  categories. Annotating multiple categories accurately can be difficult and expensive. Thus, the demand of learning on small data arises naturally to reduce the application threshold of multi-label learning. Next, we introduce some related explorations and possible future directions for this challenging setting.

Multi-label learning with limited supervision has been studied extensively. Some related approaches include semi-supervised multi-label learning [217], partial multi-label learning [218], active multi-label learning [219], multi-label learning with missing label [220] and noisy label [221], *etc.* Recently, the studies of few-shot multi-label learning [222] show the feasibility of training multi-label classifier on small data with the help of excess knowledge. These techniques sufficiently exploit the label correlation and data distribution. For example, the low rank regularization [223] is a commonly used constraint to incorporate the prior knowledge of class correlation to reduce the training data. Graph-based methods exploit the data topological information to tackle with the, *e.g.*, missing label [224], semi-supervised data [225]. Active learning methods have also been exploited to deal with the low labeling budget, some of them perform instance-level query and evaluate the uncertainty of the data based on different criteria [226], [227], while the others query the instance-label pair for fine-grained supervision [228].

Future directions may include the meta multi-label leaning. Because the label correlation prior can be crucial to the small data setting, which may be induced from historical learning experiences by the recent trending technique, *i.e.*, meta-learning. More effective active querying methods for multi-label learning are also expected to be developed.

## 8 CHALLENGING APPLICATIONS

In many real applications, the data gathering or annotation is extremely expensive, which leads to the limited training data and brings challenges to the model learning. This phenomenon brings opportunities for small data techniques. This section summarizes some of the major application areas for small data, which include computer vision, natural language processing and other topics.

### 8.1 Computer Vision

Computer vision [229] deals with the image recognition, object detection, semantic segmentation, video processing, *etc.* It has a wide range of applications in our daily life. Thanks to the powerful feature extraction ability of deep models, the state-of-the-art in computer vision has been pushed forward significantly. However, the requirement of labeled data has also been promoted to a new level due to the growing model complexity, which may be unreachable to some applications. For example, in most of medical image analysis tasks, the labeled examples are highly scarce because of the involving of expensive facilities and considerable expertise requirement for annotation. Especially for the rare diseases, both of the data and reliable annotators are limited. It is thus necessary to develop small data techniques to tackle

with this scenario. Existing explorations include designing active learning algorithms for effective queries [230], [231], transfer knowledge from related domains [232], exploiting the unlabeled data, *etc.* Nevertheless, learning on small data for medical images is still a challenging problem. Remote sensing image analysis [233] is another typical task which is lack of large amount of labeled data. It is not only because of the privacy of the data, but also the wealthy number of objects in each single image. Some studies try to tackle with this problem by proposing weakly-supervised learning methods to relax the requirement of accurate annotations [234]. Besides, novel data augmentation methods are also exploited to help the model training with limited examples [235]. Active learning is also a popular technique in the remote sensing image. The uncertainty and diversity are two commonly used criteria for remote sensing data selection [236].

Other important applications in computer vision may also include video processing [237], 3D image analysis [238], *etc.*

### 8.2 Natural Language Processing

Natural language processing (NLP) system tackles with the semantic parsing, translation, speech recognition, summarization, *etc.* for the human language. It is one of the core techniques to the man-machine interaction. However, a large numbers of labeled examples are required to train the leading NLP models, *e.g.*, Transformer [239], which can be prohibitive to some applications. For example, in the text summarization task, whose goal is to extract the key words, outline, or abstract for a long document, the annotators need to read the whole article to provide the accurate summarization. This process is usually laborious and tedious. As a result, a large scale of labeled data is usually not available in many cases. Further, due to the high dimensional feature and label spaces, learning with small data can be very challenging. Some explorations are conducted to tackle with this problem. Karn *et al.* [240] propose a few-shot learning method for text summarization, which exploits the synthetic data to pretrain the model. Data augmentation [241] has been studied to improve the model performance for few-shot text summarization learning. Bayesian active learning [242] has also been exploited to reduce the annotation cost. More effective techniques are expected to be explored in the future to tackle with this task. Another important application is the question-answering and dialogue system. It includes speech-recognition, semantic parsing, dialogue generation, and other functions, which lead to the heavy burden of data labeling. Also, due to the difficulty of the learning task, small data can usually not result in a high performance. Several active learning methods [243] are proposed to alleviate this problem. While transfer learning [244] and reinforcement learning [245] have also been explored for reducing the training data in dialogue system. However, there still exists vast space for development on the application of question-answering and dialogue system with small data.

Beyond the above topics, speech transcription [246], voice wake-up [247], machine translation [248], *etc.*, can also be important applications for small data learning.

### 8.3 Recommender System

Recommender system [249] is one of the most important applications in our daily life. It recommends possible interested contents to the users based on their historical behaviors (*e.g.*, user-item rating, transactions) and has been widely applied to the e-commerce, music, video sharing, social media platforms, *etc.* One

of the major problems of the recommender system is the cold start problem, *i.e.*, there is few or no historical data for a new user, and the data is usually private and expensive to acquire. It is thus induce the demand of developing small data techniques for the recommender system. However, the targets in this application are usually plentiful and sparse, and the feature dimension is also high, which makes the small data learning beset with difficulties. One solution to deal with this problem is introducing the extra knowledge, *e.g.*, social media [250], related source domain [251], Linked Open Data repositories [252]. Besides, some studies assume that a small questionnaire can be queried from the user to alleviate the cold start problem [253]. A related approach may be the active learning, which tries to selection the most essential user-item entries for querying [254]. Nevertheless, this problem is still open for further explorations.

#### 8.4 Time Series Data

Time series data [255] is very common in our life (*e.g.*, the temperature records, stock market trends, monitoring). It consists a sequence of successive data points. However, many time series data confront with lack of sufficient labels, incomplete sequence problems [256], and the annotation for each data is laborious. Existing studies employ active learning [257] to selectively label the most informative data to improve the model with limited budget; or exploit the unlabeled data by assigning pseudo-labels for model training, which can be implemented by label propagation [258] and model responses [259]. Further studies of learning on small data for time series data are expected to conducted.

#### 8.5 Biology

In recent years, machine learning has been widely applied to help the modern biological research [260]. Typical applications include automated genome annotation, protein binding prediction, metabolic functions prediction, *etc*. However, obtaining biology data usually requires a long-time culture (*e.g.*, cell culture), or the involving of expensive apparatuses, which bring challenges to collect large scale labeled data. Moreover, the biomedical data is often high-dimensional and sparse [261], much of them is even incomplete and biased [262]. Because of these challenges, training effective models for biological tasks can be rather difficult, especially when the labeled data is limited. Some explorations employ active learning to reduce the label acquisitions [263]; transfer learning has also been exploited to reconstruct the incomplete data [264]; graph neural network and matrix factorization techniques are applied to the disease-gene association identification task [265]. More effective approaches to deal with the small data need to be further studied.

### 9 CONCLUSION

In this paper, we firstly present a formal definition for learning on small data, and then provide theoretical guarantees for its supervised and unsupervised generalization analysis on error and label complexity under a PAC framework. From a geometric perspective, learning on small data can be characterized by the Euclidean and non-Euclidean geometric representation, where their geometric mean representations are presented and analyzed with respect to a unified expression of Fréchet mean. To optimize those geometric means, the Euclidean gradient, Riemannian gradient, and Stein gradient are investigated. Besides these technical

contents, some potential future directions of learning on small data are also summarized, and their related advanced challenging scenarios and applications are also presented and discussed.

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## APPENDIX

### Part A: Proof of Theorem 2

*Proof.* IWAL denotes a set of observations for its weighted sampling:  $\mathcal{F}_t = \{(x_1, y_1, Q_1), (x_2, y_2, Q_2), \dots, (x_t, y_t, Q_t)\}$ . The key step to prove Theorem 1 is to observe the martingale difference sequence for any pair  $f$  and  $g$  in the t-time hypothesis class  $\mathcal{H}_t$ , that is,  $\xi_t = \frac{Q_t}{p_t} (\ell(f(x_t), y_t) - \ell(g(x_t), y_t)) - (R(h) - R(g))$ , where  $f, g \in \mathcal{H}_t$ . By adopting Lemma 3 of [266], with  $\tau > 3$  and  $\delta > 0$ , we firstly know

$$\begin{aligned} & \text{var}[\xi_t | \mathcal{F}_{t-1}] \\ & \leq \mathbb{E}_{x_t} \left[ \frac{Q_t^2}{p_t^2} (\ell(f(x_t), y_t) - \ell(g(x_t), y_t)) - (R(h) - R(g))^2 | \mathcal{F}_{t-1} \right] \quad (53) \\ & \leq \mathbb{E}_{x_t} \left[ \frac{Q_t^2 p_t^2}{p_t^2} | \mathcal{F}_{t-1} \right] \\ & = \mathbb{E}_{x_t} [p_t | \mathcal{F}_{t-1}], \end{aligned}$$

and then there exists

$$\begin{aligned} & |\sum_{t=1}^T \xi_t| \\ & \leq \max_{\mathcal{H}_i, i=1,2,\dots,k} \left\{ 2 \sqrt{\sum_{t=1}^{\tau} \mathbb{E}_{x_t} [p_t | \mathcal{F}]_{t-1}}, 6 \sqrt{\log\left(\frac{8\log\tau}{\delta}\right)} \right\} \\ & \times \sqrt{\log\left(\frac{8\log\tau}{\delta}\right)}, \quad (54) \end{aligned}$$

where  $\mathbb{E}_{x_t}$  denotes the expectation over the operation on  $x_t$ . With Proposition 2 of [267], we have

$$\begin{aligned} & \sum_{t=1}^{\tau} \mathbb{E}_{x_t} [p_t | \mathcal{F}_{t-1}] \\ & \leq \left( \sum_{t=1}^{\tau} p_t \right) + 36 \log\left(\frac{(3 + \sum_{t=1}^{\tau})\tau^2}{\delta}\right) \\ & + 2 \sqrt{\left( \sum_{t=1}^{\tau} p_t \right) \log\left(\frac{(3 + \sum_{t=1}^{\tau})\tau^2}{\delta}\right)} \\ & \leq \left( \sum_{t=1}^{\tau} p_t + 6 \log\left(\frac{(3 + \sum_{t=1}^{\tau})\tau^2}{\delta}\right) \right). \quad (55) \end{aligned}$$

Then, introducing Eq. (55) to Eq. (54), with a probability at least  $1 - \delta$ , we have

$$\begin{aligned} & |\sum_{t=1}^T \xi_t| \\ & \leq \max_{\mathcal{H}_i, i=1,2,\dots,k} \left\{ \frac{2}{\tau} \left[ \sqrt{\sum_{t=1}^{\tau} p_t} + 6 \sqrt{\log\left(\frac{2(3 + \tau)\tau^2}{\delta}\right)} \right] \right. \\ & \times \left. \sqrt{\log\left(\frac{16\tau^2|\mathcal{H}_i|^2\log\tau}{\delta}\right)} \right\}. \quad (56) \end{aligned}$$

For any  $\mathcal{B}_i$ , the final hypothesis converges into  $h_{\tau}$ , which usually holds a tighter disagreement to the optimal  $h^*$ . We thus have

$R(h_{\tau}) - R(h^*) \leq |\sum_{t=1}^{\tau} \xi_t|$ . Therefore, the error disagreement bound of Theorem 1 holds. We next prove the label complexity bound of MHEAL. Following Theorem 1, there exists

$$\begin{aligned} & \mathbb{E}_{x_t} [p_t | \mathcal{F}_{t-1}] \\ & \leq 4\theta_{\text{IWAL}} K_{\ell} \times \left( R^* + \sqrt{\left( \frac{2}{t-1} \log(2t(t-1)) \right) \frac{|\mathcal{H}|^2}{\delta}} \right), \quad (57) \end{aligned}$$

where  $R^*$  denotes  $R(h^*)$ . Let  $\sqrt{\left( \frac{2}{t-1} \log(2t(t-1)) \right) \frac{|\mathcal{H}|^2}{\delta}} \propto O\left(\log\left(\frac{\tau|\mathcal{H}|}{\delta}\right)\right)$ , with the proof of Lemma 4 of [49], Eq. (55) can thus be approximated as

$$\begin{aligned} & \mathbb{E}_{x_t} [p_t | \mathcal{F}_{t-1}] \\ & \leq 4\theta_{\text{IWAL}} K_{\ell} \left( \tau R^* + O\left(R(h^*)\tau \log\left(\frac{t|\mathcal{H}|}{\delta}\right)\right) + O\left(\log^3\left(\frac{t|\mathcal{H}|}{\delta}\right)\right) \right). \quad (58) \end{aligned}$$

For any cluster  $\mathcal{B}_i$ , by adopting the proof of Theorem 2 of [49], we know

$$\begin{aligned} & \mathbb{E}_{x_t} [p_t | \mathcal{F}_{t-1}] \\ & \leq 8K_{\ell} \left\{ \left[ \sum_{j=1}^{N_i} \theta_{\text{MHEAL}} R_j^* \tau p_j \right] + \sum_{j=1}^{N_i} O\left(\sqrt{R_j^* \tau p_j \log\left[\frac{\tau|\mathcal{H}_i|N_i}{\delta}\right]}\right) \right. \\ & \left. + O\left(N_i \log^3\left(\frac{\tau|\mathcal{H}_i|N_i}{\delta}\right)\right) \right\}. \quad (59) \end{aligned}$$

Since  $\mathcal{Q} = k \times \max_{\mathcal{H}_i} \mathbb{E}_{x_t} [p_t | \mathcal{F}_{t-1}]$ , s.t.,  $i = 1, 2, \dots, k$ , our analysis of Theorem 2 on  $\mathcal{Q}$  holds. ■

### Part B: Proof of Theorem 3

*Proof.* Let  $\{\sqrt{\lambda_i} \phi_i(x)\}$  be an orthogonal base of  $\mathcal{H}$ , the kernel function can be written as:

$$K(x, y) = \sum_i^{\infty} \lambda_i \phi_i(x) \phi_i(y). \quad (60)$$

For any vector  $k_x = K(x, \cdot) \in \mathcal{H}$ , it can be expressed as a sum of orthogonal bases, i.e.,  $K(x, \cdot) = \sum_i^{\infty} \sqrt{\lambda_i} \phi_i(x) \sqrt{\lambda_i} \phi_i(\cdot)$ . May wish to assume the kernel mean  $\mu_{\mathcal{H}} = \sum_i^{\infty} \alpha_i \sqrt{\lambda_i} \phi_i(\cdot)$ , for any  $k_x \in \mathcal{H}$ , there exists

$$d_{\mathcal{H}}(k_x, \mu_{\mathcal{H}}) = \sqrt{\sum_i^{\infty} (\sqrt{\lambda_i} \phi_i(x) - \alpha_i)^2}. \quad (61)$$

Substituting Eq. (61) into Eq. (22), the kernel mean is equivalent to minimizing the following problem:

$$\min_{\mu \in \mathcal{H}} \int \sum_i^{\infty} (\sqrt{\lambda_i} \phi_i(x) - \alpha_i)^2 d\mathbb{P}(x). \quad (62)$$

The solution of Eq. (62) is  $\alpha_i = \int \sqrt{\lambda_i} \phi_i(x) d\mathbb{P}(x)$ , that is,  $\mu_{\mathcal{H}} = \sum_i^{\infty} \int \sqrt{\lambda_i} \phi_i(x) d\mathbb{P}(x) \sqrt{\lambda_i} \phi_i(\cdot)$ . To simplify  $\mu_{\mathcal{H}}$ , we next analyze the interchange of limit and integral. Let  $f_t(x) = \sum_i^t \sqrt{\lambda_i} \phi_i(x)$ , and then  $\{f_t(x)\}$  is a Cauchy sequence in  $\mathcal{H}$ . Since  $\mathcal{H}$  denotes the complete metric space, there exists  $\lim_{t \rightarrow \infty} f_t(x) = f(x) := \sum_i^{\infty} \sqrt{\lambda_i} \phi_i(x) \in \mathcal{H}$ , i.e.,

$$\lim_{t \rightarrow \infty} \|f_t - f\|_{\mathcal{H}} = 0. \quad (63)$$

The above equation shows that  $f_t(x)$  converges to  $f(x)$  in norm  $\|\cdot\|_{\mathcal{H}}$ . For RKHS, the evaluation functional  $\delta_x : \delta_x f \mapsto f(x)$  is a continuous linear functional, which means that for all  $x \in \mathcal{X}$ :

$$\begin{aligned} \lim_{t \rightarrow \infty} |f_t(x) - f(x)| &\leq \lim_{t \rightarrow \infty} |\delta_x f_t - \delta_x f| \\ &\leq \lim_{t \rightarrow \infty} \|\delta_x\| \|f_t - f\|_{\mathcal{H}} = 0. \end{aligned} \quad (64)$$

The above inequality shows that convergence in norm implies pointwise convergence in RKHS. We now consider the difference between the integral of  $f_t(x)$  and the integral of  $f(x)$ . According to the linearity and monotonicity of the Bochner integral, there exists

$$\left| \int f_t(x) d\mathbb{P}(x) - \int f(x) d\mathbb{P}(x) \right| \leq \int |f_t(x) - f(x)| d\mathbb{P}(x). \quad (65)$$

By the reverse of Fatou's lemma related to  $|f_t(x) - f(x)|$ , we have the following inequality:

$$\begin{aligned} \limsup_{t \rightarrow \infty} \int |f_t(x) - f(x)| d\mathbb{P}(x) \\ \leq \int \limsup_{t \rightarrow \infty} |f_t(x) - f(x)| d\mathbb{P}(x) = 0, \end{aligned} \quad (66)$$

which implies that the limit exists and

$$\begin{aligned} \lim_{t \rightarrow \infty} \left| \int f_t(x) d\mathbb{P}(x) - \int f(x) d\mathbb{P}(x) \right| \\ \leq \lim_{t \rightarrow \infty} \int |f_t(x) - f(x)| d\mathbb{P}(x) = 0. \end{aligned} \quad (67)$$

The above inequality shows that limit and integral is interchangeable with respect to kernel mean  $\mu_{\mathcal{H}}$ . Based on the uniqueness of limits for  $\mathcal{H}$ , the kernel mean is unique with the closed-form solution:

$$\begin{aligned} \mu_{\mathcal{H}} &= \sum_i^{\infty} \int \sqrt{\lambda_i} \phi_i(x) d\mathbb{P}(x) \sqrt{\lambda_i} \phi_i(\cdot) \\ &= \lim_{t \rightarrow \infty} \sum_i^t \int \sqrt{\lambda_i} \phi_i(x) d\mathbb{P}(x) \sqrt{\lambda_i} \phi_i(\cdot) \\ &= \lim_{t \rightarrow \infty} \int \sum_i^t \sqrt{\lambda_i} \phi_i(x) d\mathbb{P}(x) \sqrt{\lambda_i} \phi_i(\cdot) \\ &= \int \lim_{t \rightarrow \infty} \sum_i^t \sqrt{\lambda_i} \phi_i(x) d\mathbb{P}(x) \sqrt{\lambda_i} \phi_i(\cdot) \\ &= \int \sum_i^{\infty} \sqrt{\lambda_i} \phi_i(x) d\mathbb{P}(x) \sqrt{\lambda_i} \phi_i(\cdot) \\ &= \int K(x, \cdot) d\mathbb{P}(x). \end{aligned} \quad (68)$$

■

### Part C: Stein methods and SVGD algorithm

**Stein's Identity.** Given a smooth density  $p(x)$  observed on  $\mathcal{X} \subseteq \mathbb{R}^n$ , let  $A_p$  be the Stein operator,  $\varphi(x) = [\varphi_1(x), \dots, \varphi_n(x)]$  be the smooth vector function. For sufficiently regular  $\varphi$ , Stein's Identity is defined as:

$$\mathbb{E}_{x \sim p}[A_p \varphi(x)] = 0, \quad (69)$$

where

$$A_p \varphi(x) = \varphi(x) \nabla_x \log p(x)^T + \nabla_x \varphi(x). \quad (70)$$

Here  $x \sim p(x)$  denotes the continuous random variable or parameter sampled from  $\mathcal{X}$ ,  $\nabla_x \varphi(x)$  denotes the score function of  $\varphi(x)$ ,  $Q = A_p \varphi(x)$  denotes the Stein operator  $A_p$  acting on function  $\varphi$ .

**Kernelized Stein Discrepancy.** Stein Discrepancy is a discrepancy measure which can maximize violation of Stein's Identity and can be leveraged to define how different two smooth densities  $p$  and  $q$  are:

$$SD(q, p) = \max_{\varphi \in \mathcal{F}} \left\{ \left[ \mathbb{E}_{x \sim q} (\text{trace}(Q)) \right]^2 \right\}, \quad (71)$$

where  $\mathcal{F}$  denotes a set of smooth functions with bounded Lipschitz norms, it determines the discriminative capability of Stein Discrepancy. However, with [70], [268], it is computationally intractable to resolve the functional optimization problem on  $\mathcal{F}$ . To bypass this and provide a close-form solution, Liu *et al.* [269] introduce Kernelized Stein Discrepancy (KSD) which maximizes  $\varphi$  in the unit ball of a reproducing kernel Hilbert space (RKHS)  $\mathcal{H}$ . The definition of KSD is thus presented:

$$\begin{aligned} KSD(q, p) &= \max_{\varphi \in \mathcal{H}} \left\{ \left[ \mathbb{E}_{x \sim q} (\text{trace}(Q)) \right]^2 \right\} \\ &\text{s.t. } \|\varphi\|_{\mathcal{H}} \leq 1. \end{aligned} \quad (72)$$

With [69], [269], given a positive definite kernel  $k(x, x')$  :  $\mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ , the optimal solution  $\varphi(x)$  of Eq. (72) is given as:

$$\varphi(x) = \varphi_{q,p}^*(x) / \|\varphi_{q,p}^*\|_{\mathcal{H}}, \quad (73)$$

where  $\varphi_{q,p}^*(\cdot) = \mathbb{E}_{x \sim q}[A_p k(x, \cdot)]$  indicates the optimal direction for gradient descent.

With notions of SD and KSD, Liu *et al.* rethink the goal of variational inference which is defined in Eq. (28), they consider the distribution set  $\Omega$  can be obtained by smooth transforms from a tractable reference distribution  $q_0(x)$  where  $\Omega$  denotes the set of distributions of random variables which takes the form  $r = T(x)$  with density:

$$q_{[T]}(r) = q(\mathcal{R}) \cdot |\det(\nabla_r \mathcal{R})|, \quad (74)$$

where  $T : \mathcal{X} \rightarrow \mathcal{X}$  denotes a smooth transform,  $\mathcal{R} = T^{-1}(r)$  denotes the inverse map of  $T(r)$  and  $\nabla_r \mathcal{R}$  denotes the Jacobian matrix of  $\mathcal{R}$ . With the density, there should exist some restrictions for  $T$  to ensure the variational optimization in Eq. (28) feasible. For instance,  $T$  must be a one-to-one transform, its corresponding Jacobian matrix should not be computationally intractable. Also, with [72], it is hard to screen out the optimal parameters for  $T$ .

Therefore, to bypass the above restrictions and minimize the KL divergence in Eq. (28), an incremental transform  $T(x) = x + \varepsilon \varphi(x)$  is introduced, where  $\varphi(x)$  denotes the smooth function controlling the perturbation direction and  $\varepsilon$  denotes the perturbation magnitude. With the transform  $T(x)$  and the density defined in Eq. (74), we have  $q_{[T^{-1}]}(x) = q(T(x)) \cdot |\det(\nabla_x T(x))|$  and  $\text{KL}(q_{[T]} || p) = \text{KL}(q || p_{[T^{-1}]})$ . We thus have

$$\nabla_{\varepsilon} \text{KL}(q || p_{[T^{-1}]}) = \nabla_{\varepsilon} \left[ \int q(x) \log \frac{q(x)}{p_{[T^{-1}]}(x)} dx \right]. \quad (75)$$

By converting the formula of  $\text{KL}(q || p_{[T^{-1}]})$  to the corresponding mathematical expectation form,  $\nabla_{\varepsilon} \text{KL}(q || p_{[T^{-1}]})$  becomes  $-\mathbb{E}_{x \sim q} \left[ \nabla_{\varepsilon} \log (p(T(x)) |\det(\nabla_x T(x))|) \right]$ . Deriving this for-

multi further, we have

$$\nabla_{\varepsilon} \text{KL}(q||p_{[T^{-1}]}) = -\mathbb{E}_{x \sim q} [\mathcal{C} + \mathcal{D}], \quad (76)$$

where

$$\begin{aligned} \mathcal{C} &= (\nabla_{T(x)} \log p(T(x)))^\top \nabla_{\varepsilon} T(x), \\ \mathcal{D} &= (\nabla_x T(x))^{-1} \nabla_{\varepsilon} \nabla_x T(x). \end{aligned} \quad (77)$$

Besides, if  $\varepsilon = 0$ , there exists  $T(x) = x$ ,  $\nabla_{\varepsilon} T(x) = \varphi(x)$ ,  $\nabla_x T(x) = I$ , and  $\nabla_{\varepsilon} \nabla_x T(x) = \nabla_x \varphi(x)$ . With these knowledge, we present the following theorem.

**Theorem 5.** Let  $T(x) = x + \varepsilon \varphi(x)$ ,  $q_{[T]}(r)$  be the density  $r = T(x)$ , then

$$\nabla_{\varepsilon} \text{KL}(q_{[T]}||p)|_{\varepsilon=0} = -\mathbb{E}_{x \sim q} [\text{trace}(Q)], \quad (78)$$

where  $\nabla_{\varepsilon} \text{KL}(q_{[T]}||p)$  denotes the directional derivative of  $\text{KL}(q_{[T]}||p)$  when  $\varepsilon$  tends to be infinitesimal (i.e.,  $\varepsilon \rightarrow 0$ ).

Relating the definition of KSD in Eq. (72), Eq. (73), and Theorem 5, the optimal perturbation direction for Eq. (73) can be identified as  $\varphi^*(\cdot)_{q,p}$ . We thus present Lemma 2.

**Lemma 2.** Given the conditions in Theorem 5 and consider all the perturbation directions  $\varphi$  in the ball  $\mathcal{B} = \{\varphi \in \mathcal{H}^n : \|\varphi\|_{\mathcal{H}}^2 \leq \text{KSD}(q, p)\}$  of  $\mathcal{H}^n$  (i.e., RKHS), the direction of steepest descent that maximizes the negative gradient in Eq. (73) is  $\varphi_{q,p}^*$ :

$$\varphi_{q,p}^* = \mathbb{E}_{x \sim q} [k(x, \cdot) \nabla_x \log p(x) + \nabla_x k(x, \cdot)], \quad (79)$$

for which we have  $\nabla_{\varepsilon} \text{KL}(q_{[T]}||p)|_{\varepsilon=0} = -\text{KSD}(q, p)$ .