A Theory-Driven Self-Labeling Refinement Method for Contrastive Representation Learning

Pan Zhou*, Caiming Xiong*, Xiao-Tong Yuan†, Steven Hoi*

* Salesforce Research † Nanjing University of Information Science & Technology
panzhou3@gmail.com {cxiong, shoi}@salesforce.com xtyuan@nuist.edu.cn

Abstract

For an image query, unsupervised contrastive learning labels crops of the same image as positives, and other image crops as negatives. Although intuitive, such a native label assignment strategy cannot reveal the underlying semantic similarity between a query and its positives and negatives, and impairs performance, since some negatives are semantically similar to the query or even share the same semantic class as the query. In this work, we first prove that for contrastive learning, inaccurate label assignment heavily impairs its generalization for semantic instance discrimination, while accurate labels benefit its generalization. Inspired by this theory, we propose a novel self-labeling refinement approach for contrastive learning. It improves the label quality via two complementary modules: (i) self-labeling refinery (SLR) to generate accurate labels and (ii) momentum mixup (MM) to enhance similarity between query and its positive. SLR uses a positive of a query to estimate semantic similarity between a query and its positive and negatives, and combines estimated similarity with vanilla label assignment in contrastive learning to iteratively generate more accurate and informative soft labels. We theoretically show that our SLR can exactly recover the true semantic labels of label-corrupted data, and supervises networks to achieve zero prediction error on classification tasks. MM randomly combines queries and positives to increase semantic similarity between the generated virtual queries and their positives so as to improves label accuracy. Experimental results on CIFAR10, ImageNet, VOC and COCO show the effectiveness of our method. Code will be released online.

1 Introduction

Self-supervised learning (SSL) is an effective approach to learn features without manual annotations, with great success witnessed to many downstream tasks, e.g. image classification and object detection [1–7]. The methodology of SSL is to construct a pretext task that can obtain data labels via well designing the task itself, and then build a network to learn from these tasks. For instance, by constructing jigsaw puzzle [8], spatial arrangement identification [9], orientation [10], or chromatic channels [11] as a pretext task, SSL learns high-qualified features from the pretext task that can well transfer to downstream tasks. As it gets rid of the manual annotation requirement in supervised deep learning, SSL has been widely attracted increasing researching interests [1, 12].

As a leading approach in SSL, contrastive learning [1, 4, 13–16] constructs a novel instance discrimination pretext task to train a network so that the representations of different crops (augmentations) of the same instance are close, while representations of different instances are far from each other. Specifically, for an image crop query, it randomly augments the same image to obtain a positive, and view other image crops as negatives. Then it constructs a one-hot label over the positive and negatives to pull the query together with its positive and push the query away its negatives in the feature space.

Motivation. But the one-hot labels in contrastive learning are indeed inaccurate and uninformative. It is because for a query, it could be semantically similar or even more similar to some negatives.
than its positives. Indeed, some negatives even belong to the same semantic class as the query [17–19]. It holds in practice, as (i) to achieve good performance, one often uses sufficient negatives that are much more than the semantic class number, e.g. in MoCo [1], unavoidably leading to the issue on negatives; (ii) even for the same image, especially for an image containing different objects which occurs in ImageNet, random augmentations, e.g. crop, provide crops with (slightly) different semantic information, and thus some of the huge negatives could be more similar to query. So the one-hot label cannot well reveal the semantic similarity between query and its positives and “negatives”, and cannot guarantee the semantically similar samples to close each other, leading to performance degradation.

Contributions. In this work, we alleviate the above label issue, and derive some new results and alternatives for contrastive learning. Particularly, we theoretically show that inaccurate labels impair the performance of contrastive learning. Then we propose a self-labeling refinement method to obtain more accurate labels for contrastive learning. Our main contributions are highlighted below.

Our first contribution is proving that the generalization error of MoCo for instance discrimination linearly depends on the discrepancy between the estimated labels (e.g. one-hot labels) in MoCo and the true labels that really reflect semantical similarity between a query and its positives and negatives. Formally, given $n$ training queries $\mathcal{D} = \{x_i\}_{i=1}^n$ with estimated labels $\{y_i\}_{i=1}^n$ (e.g. one-hot labels in MoCo) and ground truth labels $\{\bar{y}_i\}_{i=1}^n$ on their corresponding positives and negatives, the generalization error of MoCo for instance discrimination is lower bounded by $O(\mathbb{E}_D[\|y - y^*\|_2])$, where $\mathbb{E}_D[\|y - y^*\|_2] = \frac{1}{n} \sum_{i=1}^n \|y_i - y^*_i\|_2$, and is upper bounded by $O(\sqrt{\ln(|\mathcal{F}|)) + \mathbb{E}_D[\|y - y^*\|_2]}$, where $|\mathcal{F}|$ is the covering number of the network hypotheses in MoCo. It means that the more accurate of the estimated labels $\{\bar{y}_i\}_{i=1}^n$, the better generalization of MoCo for instance discrimination.

Inspired by our theory, we propose a Self-Labeling rEfinement (SANE) method which iteratively employs the network and data themselves to generate more accurate and informative soft labels for contrastive learning. SANE has two complementary modules: (i) Self-Labeling Refinement (SLR) to explicitly generate accurate labels, and (ii) Momentum Mixup (MM) to increase similarity between query and its positive and implicitly improve label accuracy. Given a query, SLR uses its one positive to estimate semantic similarity between the query and its keys (i.e. its positive and negatives) by computing their feature similarity, since a query and its positive come from the same image and should have close similarity on the same keys. Then SLR linearly combines the estimated similarity of a query with its vanilla one-hot label in contrastive learning to iteratively generate more accurate and informative soft labels. Our strategy is that at the early training stage, one-hot label has heavy computation cost to supervise the learning of strong augmentations. In contrast, we respectively estimate the similarities of the query on all contrastive keys (its positive and negatives) and on only negatives, and linearly combines two estimated similarities with vanilla one-hot label to obtain more accurate and informative label with provable performance guarantee. Learning from noisy label, e.g. [20, 21], also uses soft labels generalized by a network to supervise
representation learning, and often focus on (semi-)supervised learning that differs from our self-supervised learning.

Two relevant works [22, 23] performed vanilla mixup on all query instances to increase data diversity. Differently, our momentum mixup mainly aims to reduce label noise, as it randomly combines one query with one positive (instead of one query) of other instances to increase the similarity between the query and its positive. Verma et al. [24] showed that mixup is a better domain-agnostic noise than Gaussian noise for positive pair construction. But they did not perform mixup on labels, which is contrast to [22, 23] and ours. See more discussion in Sec. 3.2 and empirical comparison in Sec. 4.3.

2 Inspiration: A Generalization Analysis of MoCo

In this section, we first briefly review the MoCo [1] method popularly studied for contrastive learning, and then analyze the impact of inaccurate label assignment on its generalization ability.

Review of MoCo. The MoCo method contains an online network \( f_w \) and a target network \( g_\ell \) receptively parameterized by \( w \) and \( \ell \). Both \( f_w \) and \( g_\ell \) consists of a feature encoder and a projection head (e.g. 3-layered MLP). Given a minibatch \( \{c_i\}_{i=1}^n \) at each iteration, it first randomly augments each vanilla image \( c_i \) into two views \( (x_i, \tilde{x}_i) \) and optimizes the following contrastive loss:

\[
\mathcal{L}_n(w) = -\frac{1}{s} \sum_{i=1}^n \log \left( \frac{\sigma(x_i, \tilde{x}_i)}{\sigma(x_i, \tilde{x}_i) + \sum_{j=1}^b \sigma(x_i, b_j)} \right),
\]

where \( \sigma(x_i, \tilde{x}_i) = \exp \left( -\frac{(f(x_i) - g(\tilde{x}_i))^2}{\sigma(x_i, \tilde{x}_i)} \right) \) with a temperature \( \tau \). The dictionary \( B = \{b_i\}_{i=1}^b \) denotes the negative keys of current minibatch queries \( \{x_i\}_{i=1}^n \), and is often of huge size to achieve satisfactory performance, e.g. 65,536 in MoCo. In practice, \( B \) in MoCo is updated by the minibatch features \( \{g(\tilde{x}_i)\}_{i=1}^b \) in a first-in and first-out order. By fixing \( g_\ell \) and updating \( f_w \) in Eqn. (1), MoCo pushes the query \( x_i \) away from its negative keys in dictionary \( B \) while pulling together its positive key \( \tilde{x}_i \). For \( g_\ell \), it is updated via exponential moving average, i.e. \( \ell = (1-\xi) \ell + \xi w \) with a constant \( \xi \in (0,1) \).

From Eqn. (1), one can observe that MoCo views each image as an individual class and uses one-hot label \( y_i \in \mathbb{R}^{b+1} \) (its nonzero position is at the position of its positive key) to train \( f_w \). However, as mentioned in Sec. 1, the one-hot labels cannot reveal the semantic similarity between a query \( x_i \) and its positive and negatives and thus impair representation learning. In the following, we theoretically analyze the effect of inaccurate labels to the generalization of MoCo for instance discrimination.

Generalization Analysis. We focus on analyzing MoCo in the final training stage where the sample (key) distribution in the dictionary \( B \) is almost fixed. This simplified setup is reasonable because (i) in the final training stage, the target network \( g_\ell \) almost does not change due to the very small momentum updating parameter \( \ell \), in practice and the oncoming convergence of the online network \( f_w \); (ii) dictionary is sufficient large to cover different patterns in the dataset. This fixed sample distribution simplifies the analysis, and also provides valuable insights.

Let \( \mathcal{D} = \{(x_i, \tilde{x}_i)\}_{i=1}^n \) denote the training positive pairs in MoCo sampled from an unknown distribution \( \mathcal{S} \). Moreover, the query \( x_i \) has ground truth soft label \( y^*_i \in \mathbb{R}^{b+1} \) over the key set \( B_i = \{\tilde{x}_i\cup B\} \), where the \( t \)-th entry \( y^*_i(t) \) measures the semantic similarity between \( x_i \) and the \( t \)-th key \( b_t \) in \( B_i \). In practice, given query \( x_i \) and dictionary \( B_i \), MoCo estimates an one-hot label of \( x_i \) as \( y_i \in \mathbb{R}^{b+1} \), whose first entry is one and remaining entries are zero. So \( y_i \) ignores the semantic similarity between \( x_i \) and keys in \( B_i \), and differs from \( y^*_i \). Then MoCo minimizes an empirical risk:

\[
\mathcal{Q}(f_w) = \frac{1}{n} \sum_{i=1}^n \ell(h(f_w(x_i), B_i), y_i),
\]

where \( h(f_w(x_i), B_i) = [\sigma(x_i, \tilde{x}_i), \sigma(x_i, b_1), \cdots, \sigma(x_i, b_b)] \) denotes the predicted class probability, and \( \ell(\cdot, \cdot) \) is cross-entropy loss. Ideally, one should sample sufficient pairs \( (x_i, \tilde{x}_i) \) from the distribution \( \mathcal{S} \) and use the ground truth label \( y^*_i \) of \( x_i \) to minimize the population risk:

\[
\mathcal{Q}(f_w) = \mathbb{E}_{(x_i, \tilde{x}_i) \sim \mathcal{S}} \left[ \ell(h(f_w(x_i), B_i), y^*_i) \right].
\]

Here we assume the ground truth label \( y^*_i \) is soft which is indeed more reasonable and stricter than the one-hot label setting especially for contrastive learning [25]. It is because soft label requires the networks to capture the semantic similarity between query and the instances in \( B_i \) and bring semantically similar instances together, greatly helping downstream tasks (e.g. classification) where
global semantic information is needed, while one-hot label only needs networks to distinguish each instance from others and does not consider the global semantic structures in the data. As both the data distribution $S$ and the ground truth labels are unknown, MoCo optimizes the empirical risk $\hat{Q}(f_w)$ in (11) instead of the population risk $Q(f_w)$ in (3). It is natural to ask whether $f_w$ by minimizing $\hat{Q}(f_w)$ can well perform instance discrimination task in contrastive learning, i.e., whether $f_w$ can capture the semantic similarity $(y_i^*)$ between any test sample $(x_i, \tilde{x}_i) \sim S$ and the keys (samples) in $B_i$. To solve this issue, Theorem 1 analyzes the generalization error of $f_w$ for instance discrimination.

**Theorem 1.** Suppose $\ell(h(f_w(x), B_x), y) \in [a_1, a_2]$, $\ell(\cdot, y)$ is $L_y$-Lipschitz w.r.t. $y$. Let $\mathcal{F}$ be a finite class of hypotheses $\ell(h(f_w(x), B_x), y) : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ and $|\mathcal{F}|$ be its covering number under $\|\cdot\|_\infty$ metric.

1. Let $\mathbb{E}_{D \sim S}[\|y - y^*\|_2^2] = \mathbb{E}_{D \sim S}[\frac{1}{n} \sum_{i=1}^n \|y_i - y_i^*\|_2^2]$. For any $\nu \in (0, 1)$, it holds

$$\mathbb{E}_{D \sim S}[\|y - y^*\|_2^2] \leq L_y \mathbb{E}_{D \sim S}[\|y - y^*\|_2^2] + \sqrt{\frac{2(a_2 - a_1)^2 V_D \ln(2|\mathcal{F}|/\nu)}{n}} + \frac{7(a_2 - a_1)^2 \ln(2|\mathcal{F}|/\nu)}{3(n - 1)},$$

with probability at least $1 - \nu$, where $V_D$ is the variance of $\ell(h(f(x), B_x), y^*)$ on the data $D$.

2. There exists a contrastive classification problem, a class of hypotheses $\ell(h(f_w(x), B_x), y) : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ and a constant $c_0$ such that the generalization error of $f_w$ is lower bounded

$$\mathbb{E}_{D \sim S}[\|y - y^*\|_2^2] \geq c_0 \cdot \mathbb{E}_{D \sim S}[\|y - y^*\|_2^2].$$

See its proof in Appendix C. Theorem 1 shows that for the task of learning semantic similarity between a query and its positive and negatives which is important for downstream tasks (e.g., classification), the generalization error of $f_w$ trained with the one-hot labels $y$ is upper bounded by $O(\mathbb{E}_{D \sim S}[\|y - y^*\|_2^2] + \sqrt{V_D \ln(|\mathcal{F}|)/n})$. It means that large training sample number $n$ gives small generalization error, as intuitively, model sees sufficient samples and can generalize better. The loss variance $V_D$ on the dataset $D$ measures data diversity: the larger data diversity $V_D$, the more challenging to learn a model with good generalization. Here we are particularly interested in the factor $\mathbb{E}_{D \sim S}[\|y - y^*\|_2^2]$ which reveals an important property: the higher accuracy of the training label $y$ to the ground-truth label $y^*$, the smaller generalization error. Moreover, Theorem 1 proves that there exists a contrastive classification problem such that the lower bound of generalization error depends on $\mathbb{E}_{D \sim S}[\|y - y^*\|_2^2]$. So the upper bound of generalization error is tight in terms of $\mathbb{E}_{D \sim S}[\|y - y^*\|_2^2]$. Thus, better to capture the underlying semantic similarity between query $x_i$ and samples in dictionary $B_i$ to bring semantically similar samples together and better solve downstream tasks, one should provide accurate label $y_i$ to the soft true label $y_i^*$. In the following, we introduce our solution to estimate more accurate and informative soft labels for contrastive learning.

### 3 Self-Labeling Refinement for Contrastive Learning

Our Self-Labeling Refinement (SLR) approach for contrastive learning contains (i) **Self-Labeling Refinery** (SLR for short) and (ii) **Momentum Mixup** (MM) which complementally refine noisy labels respectively from label estimation and positive pair construction. SLR uses current training model and data to estimate more accurate and informative soft labels, while MM increases similarity between virtual query and its positive, and thus improves label accuracy.

We begin by slightly modifying the instance discrimination task in MoCo. Specifically, for the query $x_i$ in the current minibatch $\{(x_i, \tilde{x}_i)\}_{i=1}^s$, we maximize its similarity to its positive sample $\tilde{x}_i$ in the key set $B = \{\tilde{x}_i\}_{i=1}^s \cup \{b_k\}_{k=1}^b$ and minimize its similarity to the remaining samples in $B$:

$$\mathcal{L}_c(w, \{(x_i, y_i)\}) = -\frac{1}{s} \sum_{i=1}^s \sum_{k=1}^{s+b} y_{ik} \log \left( \frac{\sigma(x_i, b_k)}{\sum_{l=1}^{s+b} \sigma(x_i, b_l)} \right),$$

where $b_k$ is the $k$-th sample in $B$, and $y_{ik}$ is the one-hot label of query $x_i$, whose $t$-th entry $y_{ik}$ is one. In this way, the labels of current queries $\{x_i\}_{i=1}^s$ are defined on a shared set $B$, and can be linearly combined which is key for SLR & MM. Next, we aim to improve the quality of label $y_i$ in (4) below.

#### 3.1 Self-Labeling Refinery

**Methodology.** As analyzed in Sec. 1 and 2, the one-hot labels in Eqn. (4) could not well reveal the semantic similarity between $x_i$ and the instance keys in the set $B_i$, and thus impairs good representation learning. To alleviate this issue, we introduce Self-Labeling Refinery (SLR) which employs
network and data themselves to generate more accurate and informative labels, and improves the performance of contrastive learning. Specifically, to refine the one-hot label \( y_i \) of query \( x_i \), SLR uses its positive instance \( \bar{x}_i \) to estimate the underlying semantic similarity between \( x_i \) and instances in \( B = \{ x_i \}_{i=1}^b \cup \{ b_i \}_{i=1}^b \), since \( x_i \) and \( \bar{x}_i \) come from the same image and should have close semantic similarity with instances in \( B \). Let \( b_k \) be the \( k \)-th sample in \( B \). Then at the \( t \)-th iteration, SLR first estimates the instance-class probability \( p_{ik}^t \in \mathbb{R}^{n+b} \) of \( x_i \) on the set \( B \) whose \( k \)-th entry is defined as

\[
p_{ik}^t = \alpha^{1/\tau'}(\bar{x}_i, b_k)/\sum_{i=1}^{n+b} \alpha^{1/\tau'}(\bar{x}_i, b_i), \quad (\tau' \in (0, 1]).
\]

The constant \( \tau' \) sharpens \( p_{ik}^t \) and removes some possible small noise, since smooth labels cannot well distillate their knowledge to a network [26]. Then SLR uses \( p_{ik}^t \) to approximate the semantic similarity between \( x_i \) and the instances in \( B \) and employs it as the soft label of \( x_i \) for contrastive learning.

However, since \( \bar{x}_i \) is highly similar to itself, \( p_{ik}^t \) could be much larger than others and conceals the similarity of other semantically similar instances in \( B \). To alleviate this artificial effect, SLR removes \( \bar{x}_i \) from the set \( B \) and re-estimates the similarity between \( x_i \) and the remaining instances in \( B \):

\[
q_{ik}^t = \sigma^{1/\tau'}(\bar{x}_i, b_k)/\sum_{i=1, i \neq k}^{n+b} \sigma^{1/\tau'}(\bar{x}_i, b_i), \quad q_{ii}^t = 0.
\]

Finally, SLR linearly combines the one-hot label \( y_i \) and two label estimations, i.e. \( p_i \) and \( q_i \), to obtain more accurate, robust and informative label \( \tilde{y}_i^t \) of \( x_i \) at the \( t \)-th iteration:

\[
\tilde{y}_i^t = (1 - \alpha_t - \beta_t) y_i + \alpha_t p_i^t + \beta_t q_i^t,
\]

where \( \alpha_t \) and \( \beta_t \) are two constants. In our experiments, we set \( \alpha_t = \mu \max_k p_{ik}^t/z \) and \( \beta_t = \mu \max_k q_{ik}^t/z \), where \( z = 1 + \mu \max_k p_{ik}^t + \mu \max_k q_{ik}^t \), the constants \( 1, \max_k p_{ik}^t \) and \( \max_k q_{ik}^t \) respectively denote the largest confidences of labels \( y_i, p_i \) and \( q_i \) on a certain class. Here hyperparameter \( \mu \) controls the prior confidence of \( p^t \) and \( q^t \). So SLR only has two parameters \( \tau' \) and \( \mu \) to tune.

The Benefit Analysis of Label Refinery. Now we analyze the performance of our SLR on label-corrupted data. We first describe the dataset. Let \( \{ c_i \}_{i=1}^K \subset \mathbb{R}^d \) be \( K \) vanilla samples belonging to \( K \leq K \) semantic classes, and \( \{ (x_i, y_i) \}_{i=1}^n \subset \mathbb{R}^d \times \mathbb{R} \) be the random crops of \( \{ c_i \}_{i=1}^K \). Since in practice, one often cares more the semantic class prediction performance of a model which often directly reflects the performance on the downstream tasks, we assume that the labels \( \{ y_i \}_{i=1}^n \) denote corrupted semantic-class labels. Accordingly, we will analyze whether SLR can refine the corrupted labels \( \{ y_i \}_{i=1}^n \) and whether it helps a model learn the essential semantic-class knowledge of \( \{ x_i \}_{i=1}^n \).

Finally, while allowing for multiple classes, we assume the labels are scalars and take values in \([-1, 1]\) interval for simplicity. We formally define our label-corrupted dataset below.

**Definition 1** ((\( \rho, \epsilon, \delta \))-corrupted dataset). Let \( \{ (x_i, y_i^\epsilon) \}_{i=1}^n \) denote the pairs of crops (augmentations) and ground-truth semantic labels, where crop \( x_i \) generated from the \( t \)-th sample \( c_i \) obeys \( \| x_i - c_i \|_2 \leq \epsilon \) with a constant \( \epsilon \), and \( y_i^\epsilon \in \{ y_i \}_{i=1}^n \) of \( x_i \) is the label of \( c_i \). Moreover, samples and the crops are normalized, i.e. \( \| c_i \|_2 = \| x_i \|_2 = 1 \) \( (\forall i, k) \). Each \( c_i \) has \( n_i \) crops, where \( c_i^{1/n_i} \leq n_i \leq c_i^{1/\delta} \) with two constants \( c_i^1 \) and \( c_i^{1/\delta} \). Besides, different classes are separated with a label separation \( \delta \):

\[
|\gamma_i - \gamma_k| \geq \delta, \quad \| c_i - c_k \|_2 \geq 2\epsilon, \quad (\forall i \neq k).
\]

A \((\rho, \epsilon, \delta)\)-corrupted dataset \( \{ (x_i, y_i) \}_{i=1}^n \) obeys the above conditions but with corrupted label \( \{ y_i \}_{i=1}^n \). Specifically, for each sample \( c_i \), at most \( \rho n_i \) augmentations are assigned to wrong labels in \( \{ y_i \}_{i=1}^n \). Then we study a network of one hidden layer as an example to investigate the label refining performance of our SLR. The network parameterized by \( W \in \mathbb{R}^{d \times K} \) and \( v \in \mathbb{R}^K \) is defined as

\[
x \in \mathbb{R}^d \mapsto f(W, x) = v^\top \phi(Wx),
\]

where \( \phi \) is an activation function. Following [27–29] which analyze convergence of networks or robust learning of network, we fix \( v \) to be a unit vector where half the entries are \( 1/\sqrt{K} \) and other half are \(-1/\sqrt{K}\) to simplify exposition. So we only optimize over \( W \) that contains most network parameters and will be shown to be sufficient for label refinery. Then given a \((\rho, \epsilon, \delta)\)-corrupted dataset \( \{ (x_i, y_i) \}_{i=1}^n \), at the \( t \)-iteration we train the network via minimizing the quadratic loss:

\[
\mathcal{L}_i(W) = \frac{1}{2} \sum_{i=1}^n (\tilde{y}_i^t - f(W, x_i))^2 = \frac{1}{2} \| y_i^t - f(W, X) \|_2^2.
\]
Here the label $g_i^t$ of sample $x_i$ is estimated by Eqn. (5) in which $p_i^t = f(W_t, \hat{x}_i)$ denotes predicted label by using the positive $\hat{x}_i$ of $x_i$, i.e. $||\hat{x}_i - c_i||_2 \leq \varepsilon$ if $x_i$ is augmented from vanilla sample $c_i$. We set $\beta_t = 0$ and $\tau^t = 1$ for simplicity, as (i) performing nonlinear mapping on network output greatly increases analysis difficulty; (ii) our refinery (5) is still provably sufficient to refine labels when $\beta_t = 0$ and $\tau^t = 1$. Then we update $W$ via gradient descent algorithm with a learning rate $\eta$:

$$W_{t+1} = W_t - \eta \nabla L_t(W_t).$$

Following most works on network convergence analysis [27–29], we use gradient descent and quadratic loss, since (i) gradient descent is expectation version of stochastic one and often reveals similar convergence behaviors; (ii) one can expect similar results for other losses, e.g. cross entropy, but quadratic loss gives simpler gradient computation. For analysis, we impose mild assumptions on network (6) and our SLR, which are widely used in network analysis [30–33].

**Assumption 1.** For network (6), assume $\phi$ and its first- and second-order derivatives obey $|\phi(0)|, |\phi'(z)|, |\phi''(z)| \leq \Gamma, \forall z$, and some $\Gamma \geq 1$, the entries of initialization $W_0$ obey i.i.d. $N(0, 1)$.

**Assumption 2.** Define network covariance matrix $\Sigma(C) = (CC^\top) \odot \mathbb{E}_u[\phi'(Cu)\phi'(Cu)^\top]$ where $C = [c_1 \ldots c_K]^\top$, $u \sim \mathcal{N}(0, I)$, $\odot$ is the elementwise product. Let $\lambda(C) > 0$ be the minimum eigenvalue of $\Sigma(C)$. For label refinery, assume $3\sqrt{\alpha/c} \sum_{t=0}^{T-1} |\alpha_t - \alpha_{t+1}| \leq \psi_1\|f(W_0, X) - y\|_2$ and

$$3\sqrt{\alpha/c} \sum_{t=0}^{T-1} (1 - \theta_2)\sum_{i=0}^{T-1} \epsilon |\alpha_t - \alpha_{t+1}| \leq \psi_2\|f(W_0, X) - y\|_2^2,$$

where $t_0 = \frac{c_1 K}{\eta \lambda(C)} \log \left(\frac{\sqrt{\alpha/c} \log K}{1 - \alpha_{\max}}\right)$ with three constants $\psi_1, \psi_2$ and $c_1$. Here $\alpha_{\max}$ is defined as $\alpha_{\max} = \max_{1 \leq t \leq t_0} \alpha_t$.

Assumption 1 is mild, as most differential activation functions, e.g. softplus and sigmoid, satisfy it, and the Gaussian initialization is used in practice. We assume Gaussian variance to be one for notation simplicity, but our technique is applicable to any constant variance. Assumption 2 requires that the discrepancy between $\alpha_t$ and $\alpha_{t+1}$ until some iteration number $t_0$ are bounded, which holds by setting proper $\alpha_t$. For $\lambda(C)$, many works [29–32] empirically and theoretically show $\lambda(C) > 0$. Based on these assumptions, we state our results in Theorem 2 with constants $c_1 \sim c_6$.

**Theorem 2.** Assume $(\{x_i, y_i\}_{i=1}^n)$ is a $(\rho, \varepsilon, \delta)$-corrupted dataset with noiseless labels $(\{y_i\}_{i=1}^n)$. Let $\xi = \log \frac{\lambda(C) K^{1/2}}{\rho}$. Suppose $\varepsilon$ and the number $k$ of hidden nodes satisfy $\varepsilon \leq \eta_2 \min(\frac{\lambda(C) K^{1/2}}{\rho}, \alpha_{\max})$, $k \geq \frac{C_4 K^{1/2}}{\alpha_{\max}^2 \xi \sqrt{\log K / \lambda(C)}}$. Let $\psi' = 1 + \frac{\sqrt{\xi}}{\sqrt{2}} + \sqrt{\varepsilon}$. If step size $\eta \leq \frac{K}{\eta \min \lambda(C)} \log \left(\frac{\sqrt{\alpha/c} \log K}{1 - \alpha_{\max}}\right)$ iterations, the gradient descent (7) satisfies:

(1) By defining $\xi = 4\rho + c_5 \varepsilon \psi' K^{1/2} \xi \sqrt{\log K / \lambda(C)}$ and $y^* = [y^*_1, \ldots, y^*_n]$, the discrepancy between the label $\tilde{y}^t$ estimated by our SLR (5) and the true label $y^*$ of the augmentation data $\{x_i\}_{i=1}^n$ is bounded:

$$\frac{1}{\sqrt{n}}\|\tilde{y}^t - y^*\|_2 \leq \frac{1 - \alpha_t}{\sqrt{n}} \|y - y^*\|_2 + \alpha_t \zeta,$$

where $\tilde{y}^t = [\tilde{y}_1^t, \ldots, \tilde{y}_n^t]$. Moreover, if $\rho \leq \frac{\sqrt{\xi}}{\sqrt{2}}$, $\varepsilon \leq c_6 \min(\frac{\lambda(C)^2}{\alpha_{\max}^2 K^{1/2} \xi \sqrt{\log K / \lambda(C)}}, \frac{1}{\sqrt{\xi}})$, $1 - \frac{4\delta}{\xi} \leq \alpha_t$, the estimated label $\tilde{y}^t$ predicts true label $y^*_k$ of any crop $x_i$:

$$\gamma_k^* = y^*_k \quad \text{with} \quad k^* = \text{argmin}_{1 \leq k \leq K} |y^*_k - \gamma_k|.$$

(2) By using the refined label $\tilde{y}^t$ in (5) to train network and letting $f(W_t, X) = [f(W_t, x_1), \ldots, f(W_t, x_n)]$, the error of network prediction on $\{x_i\}_{i=1}^n$ is upper bounded:

$$\frac{1}{\sqrt{n}}\|f(W_t, X) - y^*\|_2 \leq \zeta.$$

If assumptions on $\rho$ and $\varepsilon$ in (1) hold, for vanilla sample $c_k (\forall k = 1 \ldots K)$, network $f(W_t, \cdot)$ predicts the true semantic label $\gamma_k$ of its any augmentation $x$ that satisfies $||x - c_k||_2 \leq \varepsilon$:

$$\gamma_k = \gamma_k^* \quad \text{with} \quad k^* = \text{argmin}_{1 \leq i \leq K} |f(W_t, x) - \gamma_i|.$$
in Assumption 2. Typically, the performance of a network heavily relies on the data diversity even without label corruption. For instance, if two samples are nearly the same but have different labels, the learning of a network is difficult. \( \lambda(C) \) can quantify this data diversity, as one can think of \( \lambda(C) \) as a condition number associated with the network which measures the diversity of the vanilla samples \( \{c_i\}_{i=1}^{n} \). Intuitively, if there are two similar vanilla samples, \( \Sigma(C) \) is trivially rank deficient and has small minimum eigenvalue, meaning more challenges to distinguish the augmentations \( x \) generated from \( c_i \). Moreover, when the label corruption ratio \( \rho \) and the augmentation distance \( \epsilon \) are small, the label \( y_i \) estimated by our SLR can predict the true semantic label \( y_i^* \) for any crop sample \( x_i \), and thus can supervises a network to learn the essential semantic-class knowledges from \( \{x_i\}_{i=1}^{n} \).

The second result in Theorem 2 shows that by using the refined label \( y_i^* \) in our SLR (5) to train network \( f(W, \cdot) \), the error of network prediction on augmentations \( \{x_i\}_{i=1}^{n} \) can be upper bounded by \( \zeta \). Similarly, the factor \( \rho \) and \( \lambda(C) \) in \( \zeta \) respectively reflect the initial label error and the data diversity, which both reflect the learning difficulty for a model on the augmentation data \( \{(x_i, y_i)\}_{i=1}^{n} \). More importantly, our results also guarantee the test performance of the trained network \( f(W, \cdot) \).

Specifically, when the label corruption ratio \( \rho \) and sample augmentation distance \( \epsilon \) are small, for any vanilla sample \( c_k (\forall k = 1 \cdots K) \), the network \( f(W, \cdot) \) trained by our SLR can exactly predict the true semantic label \( \gamma_k \) of its any augmentation \( x \) (i.e. \( ||x - c_k||_2 \leq \epsilon \)). These results accord with Theorem 1 that shows the more accurate of training labels, the better generalization of the trained network. These results show the effectiveness of the refined labels by our method.

### 3.2 Momentum Mixup

Now we propose momentum mixup (MM) to further reduce the possible label noise in realistic data and increase the data diversity as well. Similar to vanilla mixup [34], we construct virtual instance as

\[
x_i' = \theta x_i + (1 - \theta) \bar{x}_k, \quad y_i' = \theta y_i + (1 - \theta) \bar{y}_k, \quad \theta \sim \text{Beta}(\kappa, \kappa) \in [0, 1],
\]

(8)

where \( \bar{x}_k \) is randomly sampled from the key set \( \{\bar{x}_i\}_{i=1}^{s} \), \( \bar{y}_k \) denotes the refined label by Eqn. (5), \( \text{Beta}(\kappa, \kappa) \) is a beta distribution. Here \( x_i \) and \( \bar{x}_k \) share the same label \( y_i \) on the set \( B = \{x_i\}_{i=1}^{n} \cup \{b_i\}_{i=1}^{b} \), as they come from the same instance. We call the mixup (8) as "momentum mixup", since the sample \( \bar{x}_k \) is fed into the momentum-updated network \( g_{\bar{\theta}} \), and plays a contrastive key for instance discrimination. So MM differs from the vanilla mixup used in [22, 23] where \( \bar{x}_k \) is replaced with \( x_k \) and both are fed into online network \( f_w \), and enjoys the following advantages.

Firstly, MM can improve the accuracy of the label \( y_i \) compared with vanilla mixup. For explanation, assume \( y_i \) in (8) is one-hot label. Then \( x_i \) has two positive keys \( \bar{x}_i \) and \( \bar{x}_k \) in \( B \) decided by its label \( y_i \). Accordingly, the component \( \bar{x}_k \) in \( x_i' = \theta x_i + (1 - \theta) \bar{x}_k \) directly increases the similarity between the query \( x_i' \) and its positive key \( \bar{x}_k \) in \( B \). So the label weight \( (1 - \theta) \) of label \( y_i' \) on the key \( \bar{x}_k \) to bring \( x_i' \) and \( \bar{x}_k \) together is relatively accurate, as \( x_i' \) really contains the semantic information of \( \bar{x}_k \). Meanwhile, the sum of label weights in \( y_i' \) on remaining instance in \( B \) \( \bar{x}_k \) is scaled by \( \theta \), which also scales the possible label noise on instances in \( B \). \( \bar{x}_k \) is scaled smaller due to \( \theta < 1 \). By comparison, for vanilla mixup, the label weight \( (1 - \theta) \) of label \( y_i' \) on the key \( \bar{x}_k \) does not improve label accuracy. It is because the positive pair \( x_k \) and \( \bar{x}_k \) are obtained via random augmentation, e.g. crop, and may not be semantically similar, meaning that the component \( x_k \) in \( x_i' \) could not increase similarity with \( \bar{x}_k \). So its label weight \( (1 - \theta) \) to push \( x_i' \) close to the key \( \bar{x}_k \) is not as accurate as the one in MM.

Another advantage of MM is that it allows us to use strong augmentation. As observed in [12], directly using strong augmentation in contrastive learning, e.g. MoCo, leads to performance degradation, since the instance obtained by strong augmentation often heavily differs from the one with weak augmentation. As aforementioned, the component \( \bar{x}_k \) in \( x_i' = \theta x_i + (1 - \theta) \bar{x}_k \) increases the similarity between the query \( x_i' \) and the key \( \bar{x}_k \) in \( B \), even though \( (x_i, \bar{x}_i) \) is obtained via strong augmentation. So MM could reduce the matching difficulty between positive instances.

With all the components in place, we are ready to define our proposed SANE model as follows:

\[
L(w) = (1 - \lambda)L_c(w, \{(x_i, y_i)\}) + \lambda L_c(w, \{(x_i', y_i')\}),
\]

(9)

where \( L_c(w, \{(x_i, y_i)\}) \) defined in Eqn. (4) denotes the vanilla contrastive loss with one-hot label \( y_i \), \( L_c(w, \{(x_i', y_i')\}) \) denotes the momentum mixup loss with label \( y_i' \) estimated by our self-labeling refinery (5), and \( \lambda \) is a constant. Experimental results in Sec. 4 show the effectiveness of both loss terms. See algorithm details in Algorithm 1 of Appendix B.
**Limitation Discussion.** SANE follows MoCo-like framework and hopes to obtain a more accurate soft label of a query over its positive and negatives for instance discrimination. So one limitation of SANE is that it does not apply to BYOL-alike methods [6] that only pulls positive pair together and does not require any labels. However, momentum mixup in SANE which increases the similarity of positive pair may also benefit BYOL, which is left as our future work to thoroughly test.

4 Experiments

4.1 Evaluation Results on CIFAR10 and ImageNet

**Settings.** We use ResNet50 [36] with a 3-layered MLP head for CIFAR10 [37] and ImageNet [38]. We first pretrain SANE, and then train a linear classifier on top of 2048-dimensional frozen features in ResNet50. With dictionary size 4,096, we pretrain 2,000 epochs on CIFAR10 instead of 4,000 epochs of MoCo, BYOL, and i-Mix in [23]. Dictionary size on ImageNet is 65,536. For linear classifier, we train 200/100 epochs on CIFAR10/ImageNet. See all optimizer settings in Appendix B. We use standard data augmentations in [1] for pretraining and test unless otherwise stated. E.g., for test, we perform normalization on CIFAR10, and use center crop and normalization on ImageNet. For SANE, we set $\tau = 0.2, \tau' = 0.8, \kappa = 2$ in $\Beta(\kappa, \kappa)$ on CIFAR10, and $\tau = 0.2, \tau' = 1, \kappa = 0.1$ on ImageNet. For confidence $\mu$, we increase it as $\mu_t = \mu_{t-1} - (\mu_t - \mu_{t-1}) \cos(\pi t/T) + 1)/2$ with current iteration $t$ and total training iteration $T$. We set $m_1 = 0, m_2 = 1$ on CIFAR10, and $m_1 = 0.5, m_2 = 10$ on ImageNet. For KNN on CIFAR10, its neighborhood number is 50 and its temperature is 0.05.

For CIFAR10, to fairly compare with [23], we crop each image into two views to construct the loss (9). For ImageNet, we follow CLSA [12] and train SANE in two settings. SANE-Single uses a single crop in momentum mixup loss $\mathcal{L}_c(w, ([x'_i, y'_j])$ in (9) that crops each image to a smaller size of 96 × 96, without much extra computational cost to process these small images. SANE-Multi crop each image into five sizes 224 × 224, 192 × 192, 160 × 160, 128 × 128, and 96 × 96 and averages their momentum mixup losses. This ensures a fair comparison with CLSA and SwAV. Moreover, we use strong augmentation strategy in CLSA. Specifically, for the above small image, we randomly select an operation from 14 augmentations used in CLSA, and apply it to the image with a probability of 0.5, which is repeated 5 times. We use “(strong)” to mark whether we use strong augmentations on the small images in momentum mixup loss. Thus, SANE has almost the same training cost with CLSA, i.e. about 75 (198) hours with 8 GPUs, 200 epochs, batch size of 256 for SANE-Single (-Multi). For vanilla contrastive loss on ImageNet, we always use weak augmentations. See more details of the augmentation, loss construction, and pretraining cost on CIFAR10 and ImageNet in Appendix B.

**Results.** Table 1 shows that with weak or strong augmentations, SANE always surpasses the baselines on CIFAR10. Moreover, SANE with strong (weak) augmentation improves supervised baseline by 1.0% (0.6%). Table 2 also shows that for ImageNet under weak augmentation setting, for 200 (800) epochs SANE-Multi respectively brings 0.8% (0.6%) improvements over SwAV; with 200 (800) epochs, SANE-Single also beats the runner-up MixCo (i-Mix and SimSiam). Note, BYOL outperforms SANE-Single but was trained 1,000 epochs. With strong augmentation, SANE-Single and SANE-Multi also respectively outperform CLSA-Single and CLSA-Multi. Moreover, our self-supervised accuracy 76.4% is very close to the accuracy 76.5%

| Table 1: Classification accuracy (%) | CIFAR10 dataset | KNN linear evaluation |
|-------------------------------------|-----------------|-----------------------|
| SANE-Single (strong) | 95.2 | 96.1 |
| SANE-Multi | 95.5 | 96.5 |
| Supervised [23] | | 95.5 |

| Table 2: Top-1 accuracy (%) under linear evaluation on ImageNet. |
|---------------------------------------------------------------|
| augmentation | method (200 epochs) | Top 1 | method (≥800 epochs) | Top 1 |
|---------------|---------------------|-------|---------------------|-------|
| weak          | MoCo [1]            | 60.8  | PIRL-800epochs [39] | 63.6  |
|               | SimCLR [11]         | 61.9  | MoCo v2-800epochs  | 70.0  |
|               | CPC v2 [41]         | 63.8  | SimCLR-800epochs [3] | 70.0  |
|               | PCL [1]             | 65.9  | MoCo v2-800epochs  | 71.1  |
|               | MoCo v2 [2]         | 67.5  | BYOL-1000epochs [6] | 71.3  |
|               | CO2 [29]            | 68.0  | SimSiam-800epochs [42] | 71.3  |
|               | MixCo [22]          | 68.4  | i-Mix-800epochs [23] | 71.3  |
|               | SWAV-Multi [5]      | 72.7  | SWAV-Multi-800epochs [5] | 73.3  |
|               | SANE-Single         | 70.6  | SANE-Single-800epochs | 73.0  |
|               | SANE-Multi          | 73.5  | SANE-Multi-800epochs | 75.7  |
| strong        | CLSA-Single [12]    | 69.4  | CLSA-Single-800epochs | 72.2  |
|               | CLSA-Multi [16]     | 73.1  | CLSA-Multi-800epochs | 76.2  |
|               | SANE-Single         | 70.1  | SANE-Single-800epochs | 73.5  |
|               | SANE-Multi          | 73.7  | SANE-Multi-800epochs | 76.4  |
|               | Supervised [4]      | 76.5  | Supervised [4]       | 76.5  |

| strong + JigSaw | InfoMin Aug [43] | 70.1 | InfoMin Aug-800epochs [43] | 73.0 |
| others         | InstDisc [44]      | 54.0  | BigBiGAN [45] | 56.6  |
|               | LocalAgg [46]      | 38.8  | SeLa-800epochs [47] | 61.5  |
Table 3: Transfer learning results.

| method          | classification VOC07 Accuracy | VOC07+12 COCO AP50 | object detection AP | 
|-----------------|-------------------------------|--------------------|---------------------|
| NPID++ [44]     | 76.6                          | 79.1               | —                   |
| MoCo [1]        | 79.8                          | 81.5               | —                   |
| PIRL [59]       | 81.1                          | 80.7               | —                   |
| BoWNet [45]     | 79.3                          | 81.3               | —                   |
| SimCLR [10]     | 86.4                          | —                  | —                   |
| +Mix [23]       | 85.2                          | 82.7               | —                   |
| MoCo v2 [2]     | —                             | 82.7               | —                   |
| MoCo v2 [2]     | 87.1                          | 82.5               | 42.0                |
| SWAV-Multi [5]  | 88.9                          | 82.6               | 42.1                |
| CLSA-Multi [12] | 93.6                          | 83.2               | 42.3                |
| SANE-Multi      | 92.9                          | 82.9               | 42.7                |
| SANE-Multi (strong) | 94.0                        | 83.4               | 42.4                |
| Supervised [12] | 87.5                          | 81.3               | 40.8                |

Table 4: Effects of the components in SANE with strong augmentation on CIFAR10.

| label p in (5) | label q in (5) | momentum mixup | accuracy (%) |
|---------------|----------------|----------------|--------------|
| ✓             | ✓              | ✓              | 93.7         |
| ✓             | ✓              | ✓              | 94.0         |
| ✓             | ✓              | ✓              | 94.5         |
| ✓             | ✓              | ✓              | 94.8         |
| ✓             | ✓              | ✓              | 94.9         |
| ✓             | ✓              | ✓              | 95.2         |
| ✓             | ✓              | ✓              | 95.1         |
| ✓             | ✓              | ✓              | 95.9         |

Table 5: Effects of parameter λ in SANE with strong augmentation on CIFAR10.

| regularization λ | accuracy (%) |
|------------------|--------------|
| 0                | 94.3         |
| 0.25             | 95.8         |
| 0.5              | 95.9         |
| 0.75             | 95.5         |
| 1                | 94.5         |

Table 6: Effects of various mixups on ImageNet.

|                          | MoCo+mixup | MoCo+momentum mixup |
|--------------------------|------------|---------------------|
| CIFAR10 (weak)           | 93.7       | 94.2                |
| CIFAR10 (strong)         | 93.3       | 94.8                |
| ImageNet (weak)          | 68.4 [22]  | 69.0                |

of supervised baseline, and still improves 0.2% over CLEAN-Multi even for this challenging case. These results show the superiority and robustness of SANE, thanks to its self-labeling refinery and momentum mixup which both improve label quality and thus bring semantically similar samples together.

4.2 Transfer Results on Downstream Tasks

**Settings.** We evaluate the pretrained SANE model on VOC [49] and COCO [50]. For classification, we train a linear classifier upon ResNet50 100 epochs by SGD. For object detection, we use the same protocol in [1] to fine-tune the pretrained ResNet50 based on detectron2 [51] for fairness. On VOC, we train detection head with VOC07+12 trainval data and tested on VOC07 test data. On COCO, we train the head on train2017 set and evaluate on the val2017. See optimization settings in Appendix B.

**Results.** Table 3 shows that SANE consistently outperforms the compared state-of-the-art approaches on both classification and object detection tasks, and enjoys better performance than supervised method pretrained on ImageNet. These results show the superior transferability of SANE.

4.3 Ablation Study

We train SANE 1,000 epochs on CIFAR10 to investigate the effects of each component in SANE using strong augmentation. Table 4 shows the benefits of each component, i.e. the label estimations p and q in self-labeling refinery, and momentum mixup. Table 5 shows the stable performance (robustness) of SANE on CIFAR10 when regularization parameter λ in (9) varies in a large range.

Then we compare our momentum mixup (8) with vanilla mixup in the works [22, 23]. Specifically, we use one-hot label in MoCo and replace $\tilde{x}_j$ in (8) with the query $x_j$ to obtain “MoCo+ mixup”, and ours with one-hot label can be viewed as “MoCo+momentum mixup”.

Then we train them 1,000 epochs on CIFAR10 with weak/strong augmentation, and 200 epochs on ImageNet with weak augmentations. Table 6 shows that with weak augmentation, momentum mixup always outperforms vanilla mixup in [22, 23]. Moreover, momentum mixup using strong augmentation improves its weak augmentation version, while vanilla mixup with strong augmentation suffers from performance degradation. It is because as discussed in Sec. 3.2, momentum mixup well reduces the possible label noise, especially for strong augmentations, and can enhance the performance more.

5 Conclusion

In this work, we prove the benefits of accurate labels to the generalization of contrastive learning. Inspired by this theory, we propose SANE to improve label quality in contrastive learning via self-labeling refinery and momentum mixup. The former uses the positive of a query to generate informative soft labels and combines with vanilla one-hot label to improve label quality. The latter randomly combines queries and positives to make virtual queries more similar to their corresponding positives, improving label accuracy. Experimental results testified the advantages of SANE.
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A Structure of This Document

This supplementary document contains more additional experimental details and the technical proofs of convergence results of the manuscript entitled “A Theory-Driven Self-Labeling Refinement Method for Contrastive Representation Learning”. It is structured as follows. In Appendix B, we provide more experimental details, including training algorithm, network architecture, optimizer details, loss construction and training cost of SANE. Appendix C presents the proof details of the main results, namely, Theorem 1, in Section 2, which analyzes the generalization performance of MoCo.

Next, Appendix D introduces the proof roadmap and details of the main results, i.e. Theorem 2, in Section 3.1. Since the proof framework is relatively complex, we first introduce some necessary preliminaries, including notations, concepts and assumptions that are verified in subsequent analysis in Appendix D.2.4. Then we provide the proofs of Theorem 2 in Appendix D.2. Specifically, we first introduce the proof roadmap of Theorem 2 in Appendix D.2.1. Then we present several auxiliary theories in Appendix D.2.2. Next, we prove our Theorem 2 in Appendix D.2.3. Finally, we present all proof details of auxiliary theories in Appendix D.2.4.

B More Experimental Details

Due to space limitation, we defer more experimental details to this appendix. Here we first introduce the training algorithm of SANE, and then present more setting details of optimizers, architectures, loss construction for CIFAR10 and ImageNet.

B.1 Algorithm Framework of SANE

In this subsection, we introduce the training algorithm of SANE in details, which is summarized in Algorithm 1. Same as MoCo [1] and CLSA [12], we alternatively update the online network $f_w$ and target network $g$ via SGD optimizer. Our codes are implemented based on MoCo and CLSA. The code of MoCo and CLSA satisfies “Creative Commons Attribution-NonCommercial 4.0 International Public License”.

Algorithm 1 Algorithm Framework for SANE

Input: online network $f_w$, target network $g$, dictionary $B$, temperature parameter $\tau$, momentum-update parameter $\iota$, sharpness parameter $\kappa$, prior confidence $\mu$, regularization weight $\lambda$, parameter $\kappa$ for Beta($\kappa, \kappa$), weak augmentation $T_1$, and weak or strong augmentation $T_2$

Initialization: initialize online network $f_w$, target network $g$, dictionary $B$ as MoCo.

for $i = 1 \ldots T$ do

1. sample a minibatch of vanilla samples $\{c_i\}_{i=1}^s$

2. use $T_1$ to augment $\{c_i\}_{i=1}^s$ to obtain weak augmentations $\{(x_i, \tilde{x}_i)\}_{i=1}^s$, i.e. $x_i = T_1(c_i)$ and $\tilde{x}_i = T_1(c_i)$.

3. compute feature $\{f(x_i)\}_{i=1}^s$ and $\{g(\tilde{x}_i)\}_{i=1}^s$.

4. compute the contrastive loss $\mathcal{L}_c(w,\{(x_i, y_i)\})$ in Eqn. (9)

5. use $\tilde{x}_i$ to compute the estimated labels $\tilde{y}_i$ of query $x_i$ by self-labeling refinery (5) ($\forall i = 1, \ldots, s$)

6. if using strong augmentation for momentum mixup, use $T_2$ to augment $\{c_i\}_{i=1}^s$ for obtaining strong augmentations $\{\tilde{x}_i\}_{i=1}^s$ to replace the previous $\{(x_i, \tilde{x}_i)\}_{i=1}^s$

7. use momentum mixup (8) and samples $\{(x_i, \tilde{x}_i, y_i')\}_{i=1}^s$ to obtain new virtual queries and labels $\{(x_i', y_i')\}_{i=1}^s$

8. use $\{(x_i', y_i')\}_{i=1}^s$ to compute the momentum mixup contrastive loss $\mathcal{L}_c(w,\{(x_i', y_i')\})$ in Eqn. (9)

9. update online network $f_w$ by minimizing $(1 - \lambda)\mathcal{L}_c(w,\{(x_i, y_i)\}) + \lambda \mathcal{L}_c(w,\{(x_i', y_i')\})$

10. update target network $g$ by exponential moving average

11. update the dictionary $B$ via minibatch feature $B'$ in a first-in first-out order.

end for

Output:
Experimental Settings for Linear Evaluation on CIFAR10 and ImageNet. For CIFAR10 and ImageNet, we follow [1, 4] and use ResNet50 [36] as a backbone. Then we first pretrain SANE on the corresponding training data, and then train a linear classifier on top of 2048-dimensional frozen features provided by ResNet50. For pretraining on both datasets, we use SGD with an initial learning rate 0.03 (annealed down to zero via cosine decay [52]), a momentum of 0.9, and a weight decay of $10^{-4}$. Such optimizer parameters are the same with MoCo and CLSA. Next, we pretrain 2,000 epochs on CIFAR10 with minibatch size 256 and dictionary size 4,096. For pretraining on Imagenet, the dictionary size is always 65,536; the batch size is often 256 on a cluster of 8 GPUs and is linearly scaled together with learning rate on multiple clusters. For linear classifier training, we use ADAM [53] with a learning rate of 0.01 and without weight decay to train 200 epochs on CIFAR10, and adopt SGD with an initial learning 10 (cosine decayed to zero) and a momentum of 0.9 to train 100 epochs on ImageNet. We use standard data augmentations in [1] for pretraining unless otherwise stated. Specifically, for pretraining on CIFAR10 and ImageNet, we follow MoCo and use RandomResizedCrop, ColorJitter, RandomGrayscale, GaussianBlur, RandomHorizontalFlip, and Normalization. For CIFAR10, please find its pretraining augmentation in the example^1. Except the above random augmentation, we also use the proposed momentum mixup to generate the virtual instances for constructing the momentum mixup loss.

For CIFAR10, to fairly compare with [23], we crop each image into two views to construct the loss (9). Specifically, for a minibatch of vanilla samples $\{x_i\}_{i=1}^s$, we weak augmentation $T_1$ to augment $\{x_i, \bar{x}_i\}_{i=1}^s$ to obtain weak augmentations $\{(x_i, x_i)\}_{i=1}^s$, i.e. $x_i = T_1(c_i)$ and $\bar{x}_i = T_1(c_i)$. Then same as MoCo, we can compute the contrastive loss by using $\{(x_i, x_i)\}_{i=1}^s$. Meanwhile, we use $\bar{x}_i$ to compute the soft label $\bar{y}_i$ of $x_i$ via (5). Next, we use momentum mixup (8) and samples $\{(x_i, \bar{x}_i, \bar{y}_i)\}_{i=1}^s$ to obtain new virtual queries and labels $\{(x_i', y_i')\}_{i=1}^s$, and then use $\{(x_i', y_i')\}_{i=1}^s$ to compute the momentum mixup contrastive loss $\mathcal{L}_c(w;\{(x_i', y_i')\})$ in Eqn. (9). For strong augmentation, after we compute the vanilla contrastive loss in MoCo, and then use strong augmentation to augment $\{x_i\}_{i=1}^s$ to replace $\bar{x}_i$ in $\{(x_i, \bar{x}_i, \bar{y}_i)\}_{i=1}^s$. Then we can generate virtual query instances and their labels $\{(x_i', y_i')\}_{i=1}^s$ by using $\{(x_i, \bar{x}_i, \bar{y}_i)\}_{i=1}^s$. The training cost on CIFAR10 for 2,000 epochs is about 11 days on single V100 GPU.

For ImageNet, we follow CLSA for fair comparison. For SANE-Single, we use the same way to construct the contrastive loss, and then use augmentation $T_1$ to augment $\{x_i\}_{i=1}^s$ to replace $\bar{x}_i$ in $\{(x_i, \bar{x}_i, \bar{y}_i)\}_{i=1}^s$ to construct the momentum mixup loss. Indeed, we also can do not replace $\bar{x}_i$ in $\{(x_i, \bar{x}_i, \bar{y}_i)\}_{i=1}^s$ for momentum mixup loss, which actually did not affect the performance. We do it, since SANE-Multi crops each image into five different crops for constructing momentum mixup loss, and thus SANE-Single and SANE-Multi will be more consistent, i.e. SANE-Multi uses 5 crops while SANE-Single uses one crop. For strong augmentation, we replace the augmentation $T_1$ in momentum mixup with strong augmentation, which is the same on CIFAR10. As mentioned above, to construct the momentum mixup loss, SANE-Multi crops each image into five sizes $224 \times 224$, $192 \times 192$, $160 \times 160$, $128 \times 128$, and $96 \times 96$ and averages their momentum mixup losses. For the vanilla contrastive loss, SANE-Multi uses the same way in SANE-Single to compute. In this way, SANE-Single and SANE-Multi respectively have the same settings with CLSA-Single and CLSA-Multi. Thus, ELSE has almost the same training cost with CLSA, i.e. about 75 (188) hours with 8 GPUs, 200 epochs, batch size of 256 for SANE-Single (Multi). It should be mentioned that for vanilla contrastive loss in both CLSA-Single and CLSA-Multi, we always use weak augmentations.

Transfer Evaluation Settings. We evaluate the pretrained model on ImageNet on VOC [49] and COCO [50]. For VOC, similar to linear evaluation, we train a linear classifier upon ResNet50 100 epochs by SGD with a learning rate 0.05, a momentum 0.9, batch size 256, and without weight and learning rate decay. For COCO, we adopt the same protocol in [1] to fine-tune the pretrained ResNet50 based on detector2 [51] for fairness. We evaluate the transfer ability of the cells selected on CIFAR10 by testing them on ImageNet. Following DARTS, we use momentum SGD with an initial learning 0.025 (cosine decayed to zero), a momentum of 0.9, a weight decay of $3 \times 10^{-4}$, and gradient norm clipping parameter 5.0.

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1https://colab.research.google.com/github/facebookresearch/moco/blob/colab-notebook/colab/moco_cifar10_de
C Proofs of The Results in Section 2

Lemma 1. [54] Suppose the loss ℓ is bounded by the range [a, b], namely ℓ(cef(x, w), y) ∈ [a, b]. Then let F be a finite class of hypotheses ℓ(cef(x, w), y) : X → R. Let

\[ Q_e(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i; w), y_i), \quad Q(f) = E_{(x, y) \in S} [\ell(f(x; w), y)] \]

respectively denote the empirical and population risk, where S denote the unknown data distribution and the sampled dataset D = \{(x_i, y_i)\}_{i=1}^{n} \sim S is of size n. Then for any δ ∈ (0, 1), with probability at least 1 − δ we have

\[ Q(f) \leq Q_e(f) + \sqrt{\frac{2(b-a)^2 V_D \ln(2|F|/\delta)}{n}} + \frac{7(b-a)^2 \ln(2|F|/\delta)}{3(n-1)}, \quad (10) \]

where V_D denotes the variance of the loss ℓ(cef(x; w), y) on the dataset D, and |F| denotes the covering number of F in the uniform norm \| \cdot \|_\infty.

Lemma 2. [55] For any polynomials f(x) = \sum_{i=0}^{p} a_i x^i, x \in [0,1] and \sum_{i=1}^{p} |a_i| < 1, there exists a multilayer neural network f(x) with \( O(p + \log \frac{1}{\epsilon}) \) layers, \( O(\log \frac{1}{\epsilon}) \) binary step units and \( O(p \log \frac{1}{\epsilon}) \) rectifier linear units such that \( |f(x) - f(x)| \leq \epsilon, \forall x \in [0,1] \).

Assume that function f is continuous on \([0,1]\) and \( \log \frac{1}{\epsilon} + 1 \) times differential in \((0,1)\). Let \( f^{(n)} \) denote the derivative of f of \( n-th \) order and \( \|f\| = \max_{x \in [0,1]} f(x) \). If \( \|f^{(n)}\| \leq n! \) holds for all \( n \in [\log \frac{1}{\epsilon} + 1] \), then there exists a deep network f with \( O(\log \frac{1}{\epsilon}) \) layers, \( O(\log \frac{1}{\epsilon}) \) binary step units and \( O(\log^2 \frac{1}{\epsilon}) \) rectifier linear units such that \( |f(x) - f(x)| \leq \epsilon, \forall x \in [0,1] \).

For expression power analysis of deep network, more stronger results can be found in [56–59] and all show that any function can be approximated by a deep network to arbitrary accuracy.

C.1 Proof of Theorem 1

Proof. Here we use two steps to prove our results in Theorem 1.

\[ Q(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(h(f_w(x_i), B_i), y_i), \quad (11) \]

Step 1. proof for first part results. To begin with, we first define an empirical risk \( Q_e(f) \):

\[ Q_e(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(h(f_w(x_i), B_i), y_i^*) \]

where \( Q_e(f) \) uses the ground truth label \( y_i^* \) for training. From Lemma 1, with probability at least \( 1 - \delta \), we have

\[ Q(f) \leq Q_e(f) + \sqrt{\frac{2(b-a)^2 V_D \ln(2|F|/\delta)}{n}} + \frac{7(b-a)^2 \ln(2|F|/\delta)}{3(n-1)}, \]

where \( Q(f) \) is the population risk, and \( Q_e(f) \) is the empirical risk. Both are trained with the ground truth \( y_i^* \). So the remaining work is to upper bound \( Q_e(f) \) via \( Q(f) \). Towards this end, we can bound it as follows:

\[ Q_e(f) - Q(f) = \frac{1}{n} \sum_{i=1}^{n} \left( \ell(h(f_w(x_i), B_i), y_i^*) - \ell(h(f_w(x_i), B_i), y_i) \right) \]

\[ \overset{\text{1}}{\leq} \frac{1}{n} \sum_{i=1}^{n} \left\| \nabla y \ell(h(f_w(x_i), B_i), y) \right\| \cdot \| y_i - y_i^* \|_2 \]

\[ \overset{\text{2}}{\leq} L_y E_{i \in D} \| y_i - y_i^* \|_2 \]

\[ \overset{\text{2}}{\leq} L_y E_{D \sim S} \left\| y - y^* \right\|_2, \]

where \( \overset{\text{1}}{\leq} \) holds by using \( y = y_i + \theta (y_i^* - y_i) \) for certain \( \theta \in (0,1) \); \( \overset{\text{2}}{\leq} \) holds since we use the \( L_y \)-Lipschitz property of \( \ell(h(f_w(x_i), B_i), y) \). Then combining these results together, we can obtain the desired results:

\[ |Q(f) - Q(f)| \leq L_y E_{D \sim S} \| y_i^* - y_i \|_2 + \sqrt{\frac{2(b-a)^2 V_D \ln(2|F|/\delta)}{n}} + \frac{7(b-a)^2 \ln(2|F|/\delta)}{3(n-1)}. \]
**Step 2. Proof for second part results.** Here we can construct a simple two-classification problem for clarity. Suppose we have two classes: class one with training data $D_1 = \{(x_1, x_1, y^*_1)\}^{n/2}$ and class two with training data $D_2 = \{(x_2, x_2, y^*_2)\}^{n/2}$, where $y^*_1$ denotes the ground truth label of $x_1$ on the set $B_1 = \{x_1 \cup B\}$, and $y^*_2$ denotes the ground truth label of $x_2$ on the set $B_2 = \{x_2 \cup B\}$. Both training datasets $D_1$ and $D_2$ have $\frac{n}{2}$ samples. Here we assume there is no data augmentation which means $x_1 = \bar{x}_1$ in the manuscript. In $D_1$, its samples are the same, namely $(x_1, x_1, y^*_1)$. Similarly, $D_2$ also has the same samples, namely $(x_2, x_2, y^*_2)$. Then the predicted class probability $y_{i,j}$ of sample $x_i$ on class $j$ is as follows:

\[
y_{i,j} = \frac{e^{\delta(x_i, x_i)/\tau} + \sum_{j=1}^k e^{\delta(x_i, b_j)/\tau}}{\sum_{j=1}^k e^{\delta(x_i, b_j)/\tau}}, \quad \text{(12)}
\]

where $\delta(x_i, x_i) = \sum_{s \neq i} (f(x_i), g(\bar{x}_i))$, $\tau$ denotes a temperature. For simplicity, we let dictionary $B = \{x_1, x_2\}$. In this way, we have for both ground truth labels $y^*_1$ and $y^*_2$ that satisfy $y^*_{10} = y^*_{11}$, $y^*_{10} + y^*_{11} + y^*_{21} = 1$, $y^*_{20} = y^*_{22}$, $y^*_{20} + y^*_{21} + y^*_{22} = 1$. For this setting, here we assume the training labels are denoted by $y_1$ and $y_2$. Moreover, they satisfy $y^*_{10} = y^*_{11} > 0$, $y^*_{10} + y^*_{11} + y^*_{12} = 1$, $y^*_{20} = y^*_{22} > 0$, $y^*_{20} + y^*_{21} + y^*_{22} = 1$. The reason that we do not use one-hot labels. This is because for dictionary $B = \{x_1, x_2\}$, given a sample $x_i$ ($i = 1, 2$), $x_i$ needs to predict the labels on the set \{\{x_1 \cup B\} = \{x_1, x_2\}$, where the labels are not one-hot obviously and satisfy $y^*_1 = y^*_i > 0$. In this case, we will train the model on the training data $\hat{D} = \hat{D}_1 \cup \hat{D}_2$ where $\hat{D}_1 = \{(x_1, x_1, y^*_1)\}$ and $\hat{D}_2 = \{(x_2, x_2, y^*_2)\}$. We use $\hat{y}_i$ to denote the model predicted label of $x_i$.

Then for the test samples, we assume that half of samples are $(x_1, x_1, y^*_1)$ and remaining samples are $(x_2, x_2, y^*_2)$. Then for any network $f$, we always have

\[
Q(f) - Q_e(f) = \frac{1}{n} \sum_{i=1}^n \left( \mathbb{E}[\ell(h(f_w(x_i), B_i), y^*_1)] - \mathbb{E}[\ell(h(f_w(x_i), B_i), y^*_i)] \right) = 0.
\]

Then we attempt to lower bound $Q_e(f) - \hat{Q}(f)$. Our training dataset is $\hat{D} = \hat{D}_1 \cup \hat{D}_2$ where $\hat{D}_1 = \{(x_1, x_1, y^*_1)\}$ and $\hat{D}_2 = \{(x_2, x_2, y^*_2)\}$. Then we discuss whether the network $f$ can perfectly fit the labels $(12)$ of data $\hat{D}$. For both cases, our results can hold.

**Perfectly fitting.** Network $f$ has the capacity to perfectly fit the label $\hat{y}_1$ in $\hat{D}_1$ and the label $\hat{y}_2$ in $\hat{D}_2$ when $x_1$ are different $x_2$. In this case, we have

\[
Q_e(f) - \hat{Q}(f) = \frac{1}{n} \sum_{i=1}^n \left( \ell(h(f_w(x_i), B_i), y^*_1) - \ell(h(f_w(x_i), B_i), y^*_i) \right)
\]

\[
= \frac{1}{n} \sum_{i=1}^n \sum_{s=1}^k \left( y^*_1 \log(h(f_w(x_i), B_i)) - y^*_i \log(h(f_w(x_i), B_i)) \right)
\]

\[
= \frac{1}{n} \sum_{i=1}^n \sum_{s=1}^k \left( y^*_1 - y^*_i \right) \log \left( \frac{y^*_1}{y^*_i} \right)
\]

\[
\geq \frac{1}{n} \sum_{i=1}^n \sum_{s=1}^k \left( y^*_1 - y^*_i \right) \log \left( \frac{y^*_1}{y^*_i} \right) - \frac{1}{n} \sum_{i=1}^n \sum_{s=1}^k \left( y^*_1 - y^*_i \right) \log \left( \frac{y^*_1}{y^*_i} \right)
\]

\[
= \frac{1}{6} \left[ (y^*_1 - y^*_{10}) \log(y^*_{10}) + (y^*_1 - y^*_{11}) \log(y^*_{11}) + (y^*_1 - y^*_{12}) \log(y^*_{12}) + (y^*_1 - y^*_{20}) \log(y^*_{20}) + (y^*_1 - y^*_{21}) \log(y^*_{21}) + (y^*_1 - y^*_{22}) \log(y^*_{22}) \right]
\]

\[
\geq \frac{1}{3} \left[ \frac{y^*_1 - y^*_{10}}{1 - 2y^*_{10}} + \frac{y^*_1 - y^*_{20}}{1 - 2y^*_{20}} \right],
\]

where $\oplus$ holds since $\hat{y}_1 = y^*_1$, and $\ominus$ uses $y^*_1 = y^*_y$, $y^*_1 + y^*_1 + y^*_1 = 1$, $y^*_2 = y^*_2$, $y^*_2 + y^*_2 + y^*_2 = 1$, $y^*_1 = y^*_1$, $y^*_1 + y^*_1 + y^*_1 = 1$, $y^*_2 = y^*_2$, $y^*_2 + y^*_2 + y^*_2 = 1$. Then we can choose proper values such that

\[
y^*_1 = y^*_1 > y^*_1 > \frac{1}{3}, y^*_2 > y^*_2 > y^*_2 > \frac{1}{3}.
\]
For example, we can let \( y_1 = (0.4, 0.4, 0.2), y'_1 = (0.45, 0.45, 0.1), y_2 = (0.4, 0.2, 0.4), y'_2 = (0.45, 0.1, 0.45) \). In this way, we have \((y_1 - y_0) \log \frac{y_1}{2y_0} \geq c_1(y_1 - y_0) > 0 \) and \((y_2 - y_0) \log \frac{y_2}{2y_0} \geq c_2(y_2 - y_0) > 0 \). So this means that there exists a constant \( C \) such that

\[
\mathcal{Q}_c(f) - \mathcal{Q}(f) \geq C \cdot \mathbb{E}_{i} \left[ \left\| y'_i - y_i \right\|_2 \right] = C \cdot \mathbb{E}_{D \sim S} \left[ \left\| y^* - y \right\|_2 \right].
\]

So combining the above results gives the following desired result:

\[
\mathcal{Q}(f) - \mathcal{Q}(f) \geq C \cdot \mathbb{E}_{D \sim S} \left[ \left\| y^* - y \right\|_2 \right].
\]

**Non-perfectly fitting.** From Lemma 2 (other more results in [56–59]), one can approximate any function by a deep network to arbitrary accuracy. Specifically, for the polynomial function in Eqn. (12), there exists a multilayer neural network \( f(x) \) with proper width and depth such that \( \| y_i - \bar{y}_i \|_1 \leq \epsilon \) and \( \| y_2 - \bar{y}_2 \|_1 \leq \epsilon \), where \( y_i \) and \( \bar{y}_i \) are the predicted labels of samples \( x_1 \) and \( x_2 \) by using (12). The labels \( y_1 \) and \( y_2 \) are associated with our training dataset \( D = D_1 \cup D_2 \) where \( D_1 = \{(x_1, x_1, y_1)\} \) and \( D_2 = \{(x_2, x_2, y_2)\} \). In this case, we have

\[
\mathcal{Q}_e(f) - \mathcal{Q}(f) = \frac{1}{n} \sum_{i=1}^{n} \left( \ell(h(f_w(x_i), B_1), y_i^*) - \ell(h(f_w(x_i), B_1), y_i) \right)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \sum_{s=1}^{k} \left( y_{i,s}^* \log(h(f_w(x_i), B_1)) - y_{i,s} \log(h(f_w(x_i), B_1)) \right)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \sum_{s=1}^{k} \left( y_{i,s}^* - y_{i,s} \right) \log(\bar{y}_{i,s})
\]

\[
= \frac{1}{6} \left( (y_1 - y_0) \log(\bar{y}_0) + (y_1 - y_1) \log(\bar{y}_1) + (y_2 - y_1) \log(\bar{y}_1) \right)
\]

\[
+ (y_2 - y_0) \log(\bar{y}_0) + (y_2 - y_2) \log(\bar{y}_2) + (y_2 - y_2) \log(\bar{y}_2)
\]

\[
= \frac{1}{6} \left[ (y_1 - y_0) \log(\bar{y}_0) + (y_2 - y_0) \log(\bar{y}_0) + 2(y_2 - y_0) \log(\bar{y}_0) + (y_2 - y_0) \log(\bar{y}_0) \right]
\]

\[
= \frac{1}{3} \left( (y_1 - y_0) \log \frac{\bar{y}_0}{1-2y_0} + (y_2 - y_0) \log \frac{\bar{y}_0}{1-2y_0} \right),
\]

where \( \bar{y} \) uses \( y_1 = y_1^*, y_0 = y_0 + y_1 + y_2 = 1, y_0 = y_0 + y_1 + y_2 = 1, y_0 = y_0 + y_1 + y_2 = 1. \) Then we can choose values such that \( y_1 = y_1^*, y_0 = y_0 > 1, y_0 = y_0 + y_1 + y_2 = 1 \) and \( y_0 = y_0 + y_1 + y_2 = 1, y_0 = y_0 + y_1 + y_2 = 1 \). Then we can choose proper values such that

\[
Q_e(f) - Q(f) \geq C \cdot \mathbb{E}_{i} \left[ \left\| y'_i - y_i \right\|_2 \right] = C \cdot \mathbb{E}_{D \sim S} \left[ \left\| y^* - y \right\|_2 \right].
\]

So combining the above results gives the following desired result:

\[
Q(f) - Q(f) \geq C \cdot \mathbb{E}_{D \sim S} \left[ \left\| y^* - y \right\|_2 \right].
\]

The proof is completed.

\[\square\]

## D Proof of Results in Section 3.1

In this section, we first introduce some necessary preliminaries, including notations, conceptions and assumptions that are verified in subsequent analysis in Appendix D.2.4. Then we provide the proofs of Theorem 2 in Appendix D.2. Then, we first introduce the proof roadmap in Appendix D.2.1. Then we present several auxiliary theories in Appendix D.2.2. Next, we prove our Theorem 2 in Appendix D.2.3. Finally, we present all proof details of auxiliary theories in Appendix D.2.2.
D.1 Preliminaries

D.1.1 General Model Formulation

In this section, we outline our approach to proving robustness of overparameterized neural networks. Towards this goal, we consider a general formulation where we aim to fit a general nonlinear model of the form \( x \rightarrow f(w, x) \) with \( w \in \mathbb{R}^d \) denoting the parameters of the model. For instance in the case of neural networks \( w \) represents its weights. Given a data set of \( n \) input/label pairs \( \{(x_i, y_i)\}_{i=1}^n \subset \mathbb{R}^d \times \mathbb{R} \), we fit to this data by minimizing a nonlinear least-squares loss of the form

\[
L_t(w) = \frac{1}{2} \sum_{i=1}^{n} (\hat{y}_i^t - f(w, x_i))^2.
\]

where \( \hat{y}_i^t = (1 - \alpha_t) y_i + \alpha_t p_i = (1 - \alpha_t) y_i + \alpha_t f(w_t, x_i) \) denotes the estimated label of sample \( x_i \). In Assumption 2 we assume \( \beta_t = 0 \) and \( \tau' = 1 \) for simplicity, since performing nonlinear mapping on network output greatly increases analysis difficulty. But we will show that even though \( \beta_t = 0 \) and \( \tau' = 1 \), our refinery (5) is still sufficient to refine labels. It can also be written in the more compact form

\[
L_t(w) = \frac{1}{2} \| f(w) - \hat{y}^t \|_{\ell_2}^2 \quad \text{with} \quad f(w) := \begin{bmatrix} f(w, x_1) \\ f(w, x_2) \\ \vdots \\ f(w, x_n) \end{bmatrix}.
\]

To solve this problem we run gradient descent iterations with a constant learning rate \( \eta \) starting from an initial point \( w_0 \). These iterations take the form

\[
w_{t+1} = w_t - \eta \nabla L_t(w_t) \quad \text{with} \quad \nabla L(w) = \mathcal{J}^T(w) (f(w) - \hat{y}^t).
\]

Here, \( \mathcal{J}(w) \) is the \( n \times p \) Jacobian matrix associated with the nonlinear mapping \( f \) defined via

\[
\mathcal{J}(w) = \begin{bmatrix} \frac{\partial f(w, x_1)}{\partial w} & \cdots & \frac{\partial f(w, x_n)}{\partial w} \end{bmatrix}^T.
\]

Define the \( n \)-dimensional residual vector \( r_t(w) \) and corrupted residual vector \( e_t \) where

\[
r_t(w) = \begin{bmatrix} f(x_1, w_t) - \hat{y}_1^t \\ \vdots \\ f(x_n, w_t) - \hat{y}_n^t \end{bmatrix} \quad \text{and} \quad e_t = \hat{y}^t - y^t.
\]

A key idea in our approach is that we argue that (1) in the absence of any corruption \( r(w) \) approximately lies on the subspace \( S_+ \) and (2) if the labels are corrupted by a vector \( e \), then \( e \) approximately lies on the complement space.

Throughout, \( \sigma_{\min}(\cdot) \) denotes the smallest singular value of a given matrix. We first introduce helpful definitions that will be used in our proofs. Given a matrix \( X \in \mathbb{R}^{m \times d} \) and a subspace \( \mathcal{S} \subset \mathbb{R}^m \), we define the minimum singular value of the matrix over this subspace by \( \sigma_{\min}(X, \mathcal{S}) \) which is defined as

\[
\sigma_{\min}(X, \mathcal{S}) = \sup_{\|u\|_2 = 1, U U^T = P_{\mathcal{S}}} \|U^T X\|_2.
\]

Here, \( P_{\mathcal{S}} \in \mathbb{R}^{n \times n} \) is the projection operator to the subspace. Hence, this definition essentially projects the matrix on \( \mathcal{S} \) and then takes the minimum singular value over that projected subspace.

Since augmentations are produced by using the vanilla sample \( c_t \) and the augmentation \( x \) obeys \( \|x - c_t\|_2 \leq \epsilon_t \). So in this sense, we often call the vanilla sample and its augmentations as cluster, and call the vanilla sample as cluster center.

D.1.2 Definitions and Assumptions

To begin, we define \((\epsilon, \delta)\)-clusterable dataset. As aforementioned, we often call the vanilla sample and its augmentations as cluster, and call the vanilla sample as cluster center, because augmentations are produced by using the vanilla sample \( c_t \) and the augmentation \( x \) obeys \( \|x - c_t\|_2 \leq \epsilon_t \).

**Definition 2** \((\epsilon, \delta)\)-clusterable dataset. Suppose \( \{(x_i, y_i^t)\}_{i=1}^n \) denote the pairs of augmentation and ground-truth label, where augmentation \( x_i \) generated from the \( t \)-th sample \( c_t \) obeys \( \|x - c_t\|_2 \leq \epsilon \) with a constant \( \epsilon \), and \( y_i^t \in \{\gamma_1, \gamma_2, \ldots, \gamma_K\} \) of \( x_i \) is the label of \( c_t \). Moreover, samples and its
augmentations are normalized, i.e. $\|c_i\|_2 = \|x_i\|_2 = 1$. Each vanilla sample $c_i$ has $n_i$ augmentations, where $c_1 \leq n_1 \leq c_u \leq c_0$. Moreover, the classes are separated such that $|\gamma_r - \gamma_s| \geq \delta$, $\|c_r - c_s\|_2 \geq 2\varepsilon$, $(\forall r \neq s)$, where $\delta$ is the label separation.

Our approach is based on the hypothesis that the nonlinear model has a Jacobian matrix with bimodal spectrum where few singular values are large and remaining singular values are small. This assumption is inspired by the fact that realistic datasets are clusterable in a proper, possibly nonlinear, representation space. Indeed, one may argue that one reason for using neural networks is to automate the learning of such a representation (essentially the input to the softmax layer). We formalize the notion of bimodal spectrum below.

**Assumption 3 (Bimodal Jacobian).** Let $\beta \geq \alpha > 0$ be scalars. Let $f : \mathbb{R}^p \rightarrow \mathbb{R}^n$ be a nonlinear mapping and consider a set $D \subset \mathbb{R}^p$ containing the initial point $w_0$ (i.e. $w_0 \in D$). Let $S_+ \subset \mathbb{R}^n$ be a subspace and $S_-$ be its complement. We say the mapping $f$ has a Bimodal Jacobian with respect to the complementary subspaces $S_+$ and $S_-$ as long as the following two assumptions hold for all $w \in D$.

- **Spectrum over $S_+$:** For all $v \in S_+$ with unit Euclidian norm we have
  $$\alpha \leq \left\| J^T(w)v \right\|_{\ell_2} \leq \beta.$$  

- **Spectrum over $S_-$:** For all $v \in S_-$ with unit Euclidian norm we have
  $$\left\| J^T(w)v \right\|_{\ell_2} \leq \epsilon.$$  

We will refer to $S_+$ as the signal subspace and $S_-$ as the noise subspace.

When $\epsilon << \alpha$ the Jacobian is approximately low-rank. An extreme special case of this assumption is where $\epsilon = 0$ so that the Jacobian matrix is exactly low-rank. We formalize this assumption below for later reference.

**Assumption 4 (Low-rank Jacobian).** Let $\beta \geq \alpha > 0$ be scalars. Consider a set $D \subset \mathbb{R}^p$ containing the initial point $w_0$ (i.e. $w_0 \in D$). Let $S_+ \subset \mathbb{R}^n$ be a subspace and $S_-$ be its complement. For all $w \in D$, $v \in S_+$ and $v' \in S_-$ with unit Euclidian norm, we have that

$$\alpha \leq \left\| J^T(w)v \right\|_{\ell_2} \leq \beta \quad \text{and} \quad \left\| J^T(w)v' \right\|_{\ell_2} = 0.$$  

In Theorem 7, we verify that the Jacobian matrix of real datasets indeed have a bimodal structure i.e. there are few large singular values and the remaining singular values are small which further motivate Assumption 4. This is inline with earlier papers which observed that Hessian matrices of deep networks have bimodal spectrum (approximately low-rank) [60] and is related to various results demonstrating that there are flat directions in the loss landscape [61].

Our dataset model in Definition 1 naturally has a low-rank Jacobian when $\varepsilon_0 = 0$ and each augmentation is equal to one of the $K$ centers (vanilla samples) $\{c_\ell\}_{\ell=1}^K$. In this case, the Jacobian will be at most rank $K$ since each row will be in the span of $\{\partial f(c_\ell, w) / \partial w\}_{\ell=1}^K$. The subspace $S_+$ is dictated by the membership of each cluster center (vanilla example) as follows: Let $\Lambda_\ell \subset \{1, \ldots, n\}$ be the set of coordinates $i$ such that $x_i = c_\ell$. Then, subspace is characterized by $S_+ = \{v \in \mathbb{R}^n | v_{i_1} = v_{i_2} \text{ for all } i_1, i_2 \in \Lambda_\ell \text{ and } 1 \leq \ell \leq K\}$. When $\varepsilon_0 > 0$ and the augmentation points of each cluster (vanilla sample) are not the same as the cluster when we have the bimodal Jacobian structure of Assumption 3 where over $S_-$ the spectral norm is small but nonzero.

**Definition 3 (Support subspace).** Let $\{x_i\}_{i=1}^n$ be an input dataset generated according to Definition 1. Also let $\{\tilde{x}_i\}_{i=1}^n$ be the associated vanilla samples, that is, $\tilde{x}_i = c_\ell$ iff $x_i$ is from the $\ell$th vanilla sample. We define the support subspace $S_+$ as a subspace of dimension $K$, dictated by the cluster center membership as follows. Let $\Lambda_\ell \subset \{1, \ldots, n\}$ be the set of coordinates $i$ such that $\tilde{x}_i = c_\ell$. Then, $S_+$ is characterized by $\quad S_+ = \{v \in \mathbb{R}^n | v_{i_1} = v_{i_2} \text{ for all } i_1, i_2 \in \Lambda_\ell \text{ and for all } 1 \leq \ell \leq K\}.$  

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Before we state our general result we need to discuss another assumption and definition.

**Assumption 5** (Smoothness). The Jacobian mapping $\mathcal{J}(w)$ associated to a nonlinear mapping $f : \mathbb{R}^p \to \mathbb{R}^n$ is $L$-smooth if for all $w_1, w_2 \in \mathbb{R}^p$ we have $\|\mathcal{J}(w_2) - \mathcal{J}(w_1)\| \leq L \|w_2 - w_1\|_2$.

In Theorem 7, we verify this assumption. Note that, if $\frac{\partial \mathcal{J}(w)}{\partial w}$ is continuous, the smoothness condition holds over any compact domain (albeit for a possibly large $L$.

Additionally, to connect our results to the number of corrupted labels, we introduce the notion of subspace diffusedness defined below.

**Definition 4** (Diffusedness). $S_+$ is $\zeta$ diffused if for any vector $v \in S_+$

\[ \|v\|_\infty \leq \sqrt{\zeta/n}\|v\|_2, \]

holds for some $\zeta > 0$.

We begin by defining the average Jacobian which will be used throughout our analysis.

**Definition 5** (Average Jacobian). We define the average Jacobian along the path connecting two points $x, y \in \mathbb{R}^p$ as

\[ \mathcal{J}(y, x) := \int_0^1 \mathcal{J}(x + \alpha(y - x))d\alpha. \]

**Definition 6** (Neural Net Jacobian). Given input samples $(x_i)_{i=1}^n$, form the input matrix $X = [x_1 \ldots x_n]^T \in \mathbb{R}^{n \times d}$. The Jacobian of our learning problem, i.e. $x \mapsto f(W, x) = v^T \phi(Wx)$ and $L_t(W) = \frac{1}{2} \sum_{i=1}^n (y_i - f(W, x_i))^2$, at a matrix $W$ is denoted by $\mathcal{J}(W, X) \in \mathbb{R}^{n \times k_d}$ and is given by

\[ \mathcal{J}(W, X)^T = (\text{diag}(v^T) \phi'(W \mathcal{X}^T)) \ast \mathcal{X}^T. \]

Here $\ast$ denotes the Khatri-Rao product.

### D.1.3 Auxiliary Lemmas

**Lemma 3** (Linearization of the residual). For the general problem (13) in Appendix D.1.1, we define

\[ G(w_t) = \mathcal{J}(w_{t+1}, w_t)\mathcal{J}(w_t)^T. \]

where $\mathcal{J}(w_t)$ denotes the Jacobian matrix defined in Eqn. (15), and $\mathcal{J}(w_{t+1}, w_t) = \int_0^1 \mathcal{J}(w_t + \alpha(w_{t+1} - w_t))d\alpha$ denotes the average Jacobian matrix defined in Definition (5). When using the gradient descent iterate $w_{t+1} = w_t - \eta \nabla L_t(w_t)$, then residuals

\[ \mathcal{R}_{t+1} = f(w_{t+1}) - \tilde{y}^{t+1}, \quad \mathcal{R}_t = f(w_t) - \tilde{y}^t \]

obey the following equation

\[ \mathcal{R}_{t+1} = (I - \eta G(w_t))\mathcal{R}_t + \tilde{y}^t - \tilde{y}^{t+1}. \]

**Proof.** Here we follow [29] to prove our result. Following Definition 5, denoting $r_{t+1} = f(w_{t+1}) - \tilde{y}^{t+1}$ and $r_t = f(w_t) - \tilde{y}^t$, we find that

\[ \mathcal{R}_{t+1} = r_t - f(w_t) + f(w_{t+1}) + \tilde{y}^t - \tilde{y}^{t+1} = r_t + \mathcal{J}(w_{t+1}, w_t)(w_{t+1} - w_t) + \tilde{y}^t - \tilde{y}^{t+1} = r_t - \eta \mathcal{J}(w_{t+1}, w_t)\mathcal{J}(w_t)^T r_t + \tilde{y}^t - \tilde{y}^{t+1} = (I - \eta G(w_t))r_t + \tilde{y}^t - \tilde{y}^{t+1}. \]

Using Assumption 4, one can show that sparse vectors have small projection on $S_+$.

**Lemma 4.** [29] Suppose Assumption 4 holds. If $r \in \mathbb{R}^n$ is a vector with $s$ nonzero entries, we have that

\[ \|P_{S^+}(r)\|_\infty \leq \frac{\sqrt{s}}{n}\|r\|_2, \]

where $P_{S^+}(r)$ projects $r$ onto the space $S_+$.  

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Lemma 5. For the general problem (13) in Appendix D.1.1, let \( r_t = f(w_t) - \hat{y}^t \) and \( \hat{r}_t = P_{S_+}(r_t) \).
Suppose Assumption 4 holds and \( \eta \leq \frac{1}{\beta^2} \). If \( \|w_t - w_0\|_2 + \frac{\|\hat{r}_t\|_2}{\alpha} \leq \frac{4(1 + \psi)}{\alpha} \|r_0\|_2 \), then

\[
 w_{t+1} \in D = \{ w \in \mathbb{R}^p \mid \|w - w_0\|_2 \leq \frac{4(1 + \psi)}{\alpha} \|r_0\|_2 \}.
\]

Proof. Since range space of Jacobian is in \( S_+ \) and \( \eta \leq 1/\beta^2 \), we can easily obtain

\[
\|w_{t+1} - w_t\|_2 = \eta \|J^T(w_t) (f(w_t) - \hat{y}^t)\|_2
\]
\[
\leq (1) \eta \|J^T(w_t)(P_{S_+}(f(w_t) - \hat{y}^t))\|_2
\]
\[
\leq (2) \eta \|J^T(w_t)\hat{r}_t\|_2
\]
\[
\leq (3) \eta \beta \|\hat{r}_t\|_2
\]
\[
\leq (4) \|\hat{r}_t\|_2 / \beta
\]
\[
\leq (5) \|\hat{r}_t\|_2 / \alpha
\]

In the above, \( 1 \) follows from the fact that row range space of Jacobian is subset of \( S_+ \) via Assumption 4. \( 2 \) follows from the definition of \( \hat{r}_t = P_{S_+}(f(w_t) - \hat{y}^t) \). \( 3 \) follows from the upper bound on the spectral norm of the Jacobian over \( D \) per Assumption 4. \( 4 \) from the fact that \( \eta \leq 1/\beta^2 \). \( 5 \) from \( \alpha \leq \beta \). The latter combined with the triangular inequality and the assumption

\[
\|w_{t+1} - w_0\|_2 \leq \|w_{t+1} - w_t\|_2 + \|w_0 - w_t\|_2 \leq \|w_t - w_0\|_2 + \frac{\|\hat{r}_t\|_2}{\alpha} \leq \frac{4(1 + \psi)}{\alpha} \|r_0\|_2,
\]

concluding the proof of \( r_{t+1} \in D \). □

Lemma 6. [29] Let \( P_{S_+} \in \mathbb{R}^{n \times n} \) be the projection matrix to \( S_+ \) i.e. it is a positive semi-definite matrix whose eigenvectors over \( S_+ \) is 1 and its complement is 0. Let \( r_t = f(w_t) - y_t, \hat{r}_t = P_{S_+}(r_t) \), and \( G(w_t) = J(w_{t+1}, w_t)J(w_t)^T \). Suppose Assumptions 4 and 5 hold, the learning rate \( \eta \) satisfies \( \eta \leq \frac{\alpha}{\beta \|r_0\|_2}, \|\hat{r}_t\|_2 \leq \|\hat{r}_0\|_2 \), then it holds

\[
\beta^2 P_{S_+} \succeq G(w_t) \succeq \frac{1}{2} J(w_t)J(w_t)^T \succeq \frac{\alpha^2}{2} P_{S_+}.
\]

In the above context, we focus on introducing theoretical results for the general problem (13) in Appendix D.1.1. Now we introduce lemmas and theories for our network learning problem, i.e. \( x \mapsto f(W, x) = v^T \phi(Wx) \) and \( L_t(W) = \frac{1}{2} \sum_{i=1}^n (\hat{y}_i - f(W, x_i))^2 \) used in our manuscript. Specifically, we introduce some theoretical results in [62] and characterizes three key properties of the neural network Jacobian. These are smoothness, spectral norm, and minimum singular value at initialization which correspond to Lemmas 6.6, 6.7, and 6.8 in that paper.

Theorem 3 (Jacobian Properties at Cluster Center). [62] Suppose \( X = [x_1 \ldots x_n]^T \in \mathbb{R}^{n \times d} \) be an input dataset satisfying \( \lambda(X) > 0 \), where \( \lambda(X) \) denotes the smallest eigenvalue of matrix \( X \). Suppose \( |\phi'|, |\phi''| \leq \Gamma \) where \( \phi' \) and \( \phi'' \) respectively denotes the first and second order derivatives. The Jacobian mapping with respect to the input-to-hidden weights obey the following properties. Let \( J(W, X) \) denote the neural net Jacobian defined in Definition 6.

1. Smoothness is bounded by

\[
\|J(\tilde{W}, X) - J(W, X)\| \leq \frac{\Gamma}{\sqrt{k}} \|X\| \|\tilde{W} - W\|_F \quad \text{for all } \tilde{W}, W \in \mathbb{R}^{k \times d}.
\]

2. Top singular value is bounded by

\[
\|J(W, X)\| \leq \Gamma \|X\|.
\]
(3) Let $C > 0$ be an absolute constant. As long as

$$k \geq \frac{C T^2 \log n \|X\|^2}{\lambda(X)}$$

At random Gaussian initialization $W_0 \sim \mathcal{N}(0,1)^{k \times d}$, with probability at least $1 - 1/K^{100}$, we have

$$\sigma_{\min}(\mathcal{J}(W_0, X)) \geq \sqrt{\lambda(X)/2}.$$ 

The following theorem states the properties of the Jacobian at the cluster center matrix which is rank $K$ between noiseless and noisy labels satisfy the bound

$$\sigma_{\min}(\mathcal{J}(W, X)) \geq \sqrt{\lambda(X)/2}.$$ 

Theorem 4 (Jacobian Properties at Cluster Center). [29] Let input samples $(x_i)_{i=1}^n$ be generated according to $(\epsilon_0, \delta)$ clusterable dataset model of Definition 2. Define $X = [x_1 \ldots x_n]^T$ and $C = [c_1 \ldots c_k]^T$. Let $S_+$ be the support space and $(\tilde{x}_i)_{i=1}^n$ be the associated clean dataset as described by Definition 3. Set $\tilde{X} = [\tilde{x}_1 \ldots \tilde{x}_n]^T$. Assume $|\phi'|, |\phi''| \leq \Gamma$ and $\lambda(C) > 0$. Let $\mathcal{J}(W, X)$ denote the neural net Jacobian defined in Definition 6. The Jacobian mapping at $\tilde{X}$ with respect to the input-to-hidden weights obey the following properties.

1. Smoothness is bounded by

$$\left\| J(\tilde{W}, \tilde{X}) - J(W, X) \right\| \leq \Gamma \sqrt{\frac{\text{Cup}_n}{kK}} \|C\| \left\| \tilde{W} - W \right\|_F \quad \text{for all} \quad \tilde{W}, W \in \mathbb{R}^{k \times d}.$$ 

2. Top singular value is bounded by

$$\left\| J(W, \tilde{X}) \right\| \leq \sqrt{\frac{\text{Cup}_n}{K}} \|C\|.$$ 

3. As long as

$$k \geq \frac{C T^2 \log K \|C\|^2}{\lambda(K)}$$

At random Gaussian initialization $W_0 \sim \mathcal{N}(0,1)^{k \times d}$, with probability at least $1 - 1/K^{100}$, we have

$$\sigma_{\min}(\mathcal{J}(W_0, \tilde{X}), S_+) \geq \sqrt{\frac{\text{Cup}_n M(C)}{2K}}.$$ 

4. The range space obeys range$(\mathcal{J}(W_0, \tilde{X})) \subset S_+$ where $S_+$ is given by Definition 3.

Lemma 7 (Upper bound on initial misfit). [29] Consider a one-hidden layer neural network model of the form $x \mapsto v^T \phi(W x)$ where the activation $\phi$ has bounded derivatives obeying $|\phi(0)|, |\phi'(z)| \leq \Gamma$. Suppose entries of $v \in \mathbb{R}^k$ are half $1/\sqrt{k}$ and half $-1/\sqrt{k}$ so that $\|v\|_2 = 1$. Also assume we have $n$ data points $x_1, x_2, \ldots, x_n \in \mathbb{R}^d$ with unit euclidean norm ($\|x_i\|_2 = 1$) aggregated as rows of a matrix $X \in \mathbb{R}^{n \times d}$ and the corresponding labels given by $y \in \mathbb{R}^n$ generated according to $(\rho, \epsilon = 0, \delta)$ noisy dataset (Definition 1). Then for $W_0 \in \mathbb{R}^{k \times d}$ with i.i.d. $\mathcal{N}(0,1)$ entries

$$\|v^T \phi(W_0 X^T) - y\|_2 \leq O\left( \Gamma \sqrt{n \log K} \right),$$

holds with probability at least $1 - K^{-100}$.

Then we introduce a lemma regarding the projection of label noise on the vanilla sample (cluster) induced subspace. Since augmentations are produced by using the vanilla sample $c_i$ and the augmentation $a$ obeys $\|x - c_i\|_2 \leq \epsilon_0$. So in this sense, we sometimes call the vanilla sample and its augmentations as cluster, and call the vanilla sample as cluster center.

Lemma 8. [29] Let $\{ (x_i, y_i) \}_{i=1}^n$ be an $(\rho, \epsilon = 0, \delta)$ clusterable noisy dataset as described in Definition 1. Let $\{y_i^*\}_{i=1}^n$ be the corresponding ground truth labels. Let $\mathcal{J}(W, C)$ be the Jacobian at the cluster center matrix which is rank $K$ and $S_+$ be its column space. Then, the difference between noiseless and noisy labels satisfy the bound

$$\|P_{S_+}(y - y^*)\|_\infty \leq 2\rho.$$
Theorem 5. [29] Assume \(|\phi|, |\phi'| \leq \Gamma \text{ and } k \gtrsim d\). Suppose \(W_0 \sim \mathcal{N}(0,1)\). Let \(e_1, \ldots, e_K\) be cluster centers. Then, with probability at least \(1 - 2e^{-(k+d)} - Ke^{-10kd}\) over \(W_0\), any matrix \(W\) satisfying \(\|W - W_0\|_F \lesssim \sqrt{k}\) satisfies the following. For all \(1 \leq i \leq K\),

\[
\sup_{\|x - e_i\|_2, \|\tilde{x} - e_i\|_2 \leq \epsilon} |f(W, x) - f(W, \tilde{x})| \leq C\Gamma \epsilon (\|W - W_0\| + \sqrt{d}).
\]

Lemma 9 (Perturbed Jacobian Distance). [29] Let \(X = [x_1 \ldots x_n]^T\) be the input matrix obtained from Definition 1. Let \(\tilde{X}\) be the noiseless inputs where \(\tilde{x}_i\) is the cluster center corresponding to \(x_i\). Let \(\mathcal{J}(W, X)\) denote the neural net Jacobian defined in Definition 6 and define \(\mathcal{J}(W_1, W_2, X) = \int_0^1 \mathcal{J}(\alpha W_1 + (1 - \alpha) W_2, X) d\alpha\). Given weight matrices \(W_1, W_2, \tilde{W}_1, \tilde{W}_2\), we have that

\[
\|\mathcal{J}(W, X) - \mathcal{J}(\tilde{W}, \tilde{X})\| \leq \Gamma \sqrt{n} \left( \frac{\|\tilde{W} - W\|_F}{\sqrt{k}} + \epsilon \right).
\]

and

\[
\|\mathcal{J}(W_1, W_2, X) - \mathcal{J}(\tilde{W}_1, \tilde{W}_2, \tilde{X})\| \leq \Gamma \sqrt{n} \left( \frac{\|W_1 - W_2\|_F}{2\sqrt{k}} + \frac{\|\tilde{W}_2 - \tilde{W}_2\|_F}{\sqrt{k}} + \epsilon \right).
\]

D.2 Proof of Theorem 2

The subsection has four parts. In the first part, we introduce the proof roadmap in Appendix D.2.1. Then in the second part, we present several auxiliary theories in Appendix D.2.2. Next, we prove our Theorem 2 in Appendix D.2.3. Finally, we present all proof details of auxiliary theories in Appendix D.2.2.

D.2.1 Proof roadmap

Before proving Theorem 2, we first briefly introduce our main idea. In the first step, we analyze the general model introduced in Appendix D.1.1. For the solution \(w_t\) at the \(t\)-th iteration, Theorem 6 proves that (1) the distance of \(\|w_t - w_0\|_2\) can be upper bounded; (2) both residual \(\|P_{S_t} f(w_t) - \hat{y}\|_2\) and \(\|f(w_t) - y^*\|_\infty\) can be upper bound. Result (1) means that the gradient descent algorithm gives solutions in a ball around the initialization \(w_0\), and helps us verify our assumptions, e.g. Assumptions 5 and 4 and upper bound some variables in our analysis. Results (2) directly bound the label estimation error which plays key role in subsequent analysis.

In the second step, we prove Theorem 7 for the perfectly clustered data \((e_0 = 0)\) by using Theorem 6. We consider \(e_0 \to 0\) which means that the input data set is perfectly clean. In this setting, let \(\tilde{X} = [\tilde{x}_1, \ldots, \tilde{x}_n]\) be the clean input sample matrix obtained by mapping \(x_i\) to its associated cluster center, i.e. \(\tilde{x}_i = c_{t}\) if \(x_i\) belongs to the \(t\)-th cluster. In this way, we update network parameter \(\tilde{W}_t\) as follows:

\[
\tilde{W}_{t+1} = \tilde{W}_t - \nabla \tilde{L}_t(\tilde{W}_t) \quad \text{where} \quad \tilde{L}_t(\tilde{W}) = \frac{1}{2} \sum_{i=1}^n (y_{ti} - f(\tilde{W}, \tilde{x}_i))^2
\]

Theorem 7 shows that for neural networks, our method still can upper bound the distance \(\|\tilde{W}_t - W_0\|_F\) and the residuals \(\|f(\tilde{W}_t) - \tilde{y}\|_\infty\) if the network, learning rate, the weight \(\alpha_t\) for refining label satisfy certain conditions.

In the third step, we consider the realistic setting, where we update the parameters on the corrupted data \(X = [x_1, \ldots, x_n]\) as follows:

\[
W_{t+1} = W_t - \eta \nabla L_t(W_t) \quad \text{where} \quad L_t(W) = \frac{1}{2} \sum_{i=1}^n (y_{ti} - f(W, x_i))^2.
\]

Then to upper bound \(\|f(W_t) - \tilde{y}\|_\infty\) which measures the error between the predicted label \(f(W_t)\) and the ground truth label \(\tilde{y}\), we upper bound \(\|f(W_t, X) - f(W_t, \tilde{X})\|_2\) and \(\|W_t - \tilde{W}_t\|_F\). These results are formally stated in Theorem 8.

In the fourth step, we combine the above results together. Specifically, Theorem 7 upper bounds the residuals \(\|f(\tilde{W}_t, \tilde{X}) - \tilde{y}\|_\infty\) and Theorem 8 upper bounds \(\|f(W_t, X) - f(W_t, \tilde{X})\|_2\). So combining
these two results and other results in Theorem 7 & 8, we can upper bound \( \|f(W_t, X) - \bar{y}\|_\infty \) which is our desired results. At the same time, by using similar method, we can also bound the label estimation error by our self-labeling refinery, since \( \|\bar{y} - y^*\|_2 \leq \|f(w) - \bar{y}\|_2 \leq (1 - \alpha t)\|y - f(w) - y^*\|_2\). The term \( \|y - y^*\|_2 \) denotes the initial label error and can be bounded by a factor related to \( \rho \), while the second term is well upper bounded by the above results.

It should be note that our proof framework follows the recent works [28, 29] which shows that gradient descent is robust to label corruptions. The main difference is that this work uses the label estimation \( \bar{y} = \alpha_t y + (1 - \alpha_t)f(w) \) and minimizes the squared loss, while both works [28, 29] use the corrupted label \( \tilde{y} \) and then minimize the squared loss. By comparison, our method is much more complicated and gives different proofs.

D.2.2 Auxiliary Theories

The following theorem is to analyze the general model introduced in Appendix D.1.1. It guarantees that the estimated label by our method is close to the ground truth label when the Jacobian mapping is exactly low-rank. By using this results, one can obtain Theorem 7 for the perfectly clustered data \((e_0 = 0)\) which will be stated later.

**Theorem 6** (Gradient descent with label corruption). Consider a nonlinear least squares problem of the form \( L_c(w) = \frac{1}{2} \|f(w) - \bar{y}\|_2^2 \) with the nonlinear mapping \( f : \mathbb{R}^p \to \mathbb{R}^n \) obeying assumptions 4 and 5 over a unit Euclidean ball of radius \( \frac{d(1 + \psi)}{\alpha} \|f(w_0) - \bar{y}\|_2 \) around an initial point \( w_0 \) and \( y = [y_1 \ldots y_n] \in \mathbb{R}^n \) denoting the corrupted labels. We also assume \( \alpha_t \geq 1 - \frac{a^2}{4 \delta^2} \) and 
\[
2\sqrt{\pi} \lim_{t \to \infty} \sum_{t=0}^{t} |\alpha_t - \alpha_{t+1}| \leq \psi_1 \|f(w_0) - \bar{y}\|_2.
\]
Also let \( y^* = [y_1^* \ldots y_n^*] \in \mathbb{R}^n \) denote the ground truth labels and \( e = y - y^* \) the corruption. Furthermore, suppose the initial residual \( f(w_0) - \bar{y} \) with respect to the uncorrupted labels obey \( f(w_0) - y^* \in S_+ \). Then, running gradient descent updates of the from (14) with a learning rate \( \eta \leq \frac{1}{2\sqrt{\pi}} \min \left(1, \frac{\alpha^2}{4 \delta^2} \right) \), all iterates obey
\[
\|w_t - w_0\|_2 \leq \frac{4\|r_0\|_2}{\alpha} + 2\sqrt{\pi} \lim_{t \to \infty} \sum_{t=0}^{t} |\alpha_t - \alpha_{t+1}| \leq \frac{4\|f(w_0) - \bar{y}\|_2}{\alpha},
\]
and
\[
\|\tilde{w}_t\|_2 \leq \left(1 - \frac{\eta \alpha^2}{4}\right)^t \|\tilde{w}_0\|_2 + 2\sqrt{\pi} \sum_{t=0}^{t-1} \left(1 - \frac{\eta \alpha^2}{4}\right)^{t-i} |\alpha_i - \alpha_{i+1}|,
\]
where \( r_t = f(w_t) - \bar{y} \) and let \( r_0 = f(w_0) - \bar{y} \) be the initial residual, and \( \tilde{w}_t = \mathcal{P}_{S_+}(r_t) \). Furthermore, assume \( \nu > 0 \) is a precision level obeying \( \nu \geq \|\mathcal{P}_{S_+}(e)\|_\infty \). Then, after \( t \geq \frac{5}{\nu \eta} \log \left(\frac{\|f(w_0) - \bar{y}\|_2}{\|\mathcal{P}_{S_+}(e)\|_\infty}\right) \) iterations where \( \alpha_{max} = \max \alpha_t \), \( w_t \) achieves the following error bound with respect to the true labels
\[
\|f(w_t) - y^*\|_\infty \leq 2\nu + \frac{2\sqrt{\pi}}{1 - \alpha_t} \sum_{i=0}^{t-1} \left(1 - \frac{\eta \alpha^2}{4}\right)^{t-i} |\alpha_i - \alpha_{i+1}|.
\]
Furthermore, if \( e \) has at most \( s \) nonzeros and \( S_+ \) is \( \zeta \) diffused per Definition 4, then using \( \nu = \|\mathcal{P}_{S_+}(e)\|_\infty \)
\[
\|f(w_t) - y^*\|_\infty \leq 2\|\mathcal{P}_{S_+}(e)\|_\infty + \frac{2\sqrt{\pi}}{1 - \alpha_t} \sum_{i=0}^{t-1} \left(1 - \frac{\eta \alpha^2}{4}\right)^{t-i} |\alpha_i - \alpha_{i+1}| \leq \frac{\sqrt{\pi}}{\eta} \|e\|_2 + \frac{2\sqrt{\pi}}{1 - \alpha_t} \sum_{i=0}^{t-1} \left(1 - \frac{\eta \alpha^2}{4}\right)^{t-i} |\alpha_i - \alpha_{i+1}|,
\]
where \( \mathcal{P}_{S_+}(e) \) denotes projection of \( e \) on \( S_+ \).

See its proof in Appendix D.2.5. This result shows that when the Jacobian of the nonlinear mapping is low-rank, our method enjoys two good properties.

For the solution \( w_t \) at the \( t \)-th iteration, (1) the distance of \( \|w_t - w_0\|_2 \) can be upper bounded; (2) both residual \( \|\mathcal{P}_{S_+}(f(w_t) - y_t)\|_2 \) and \( \|f(w_t) - \bar{y}\|_\infty \) can be upper bound. Result (1) means that
the gradient descent algorithm gives solutions in a ball around the initialization \( w_0 \), and helps us verify our assumptions, e.g. Assumptions 5 and 4 and upper bound some variables in our analysis. Results (2) directly bound the label estimation error which plays key role in subsequent analysis. This theorem is the key result that allows us to prove Theorem 7 when the data points are perfectly clustered \( (\epsilon_0 = 0) \). Furthermore, this theorem when combined with a perturbation analysis allows us to deal with data that is not perfectly clustered \( (\epsilon_0 > 0) \) and to conclude the recovery ability of our method (Theorem 2).

When \( \epsilon_0 \rightarrow 0 \) which means that the input data set is perfectly clustered, our method can be expected to exactly recover the ground truth label by using neural networks.

**Theorem 7** (Training with perfectly clustered data). Consider the setting and assumptions of Theorem 6 with \( \epsilon_0 = 0 \). Starting from an initial weight matrix \( W_0 \) selected at random with i.i.d. \( \mathcal{N}(0, 1) \) entries we run gradient descent updates of the form \( W_{t+1} = W_t - \eta \nabla L_t(W_t) \) on the least-squares loss in the manuscript with step size \( \eta \leq \frac{K}{2c \epsilon_0 n^2 \| C \|^2} \). Furthermore, assume the number of hidden nodes obey

\[
k \geq C(1 + \psi_1)^2 \Gamma^4 \frac{K \log(K)\| C \|^2}{\lambda(C)^2},
\]

with \( \lambda(C) \) is the minimum eigenvalue of \( \Sigma(C) \) in Assumption 2. Then, with probability at least \( 1 - 2/K^{100} \) over randomly initialized \( W_0 \), the iterates \( W_t \) obey the following properties.

1. The distance to initial point \( W_0 \) is upper bounded by

\[
\|W_t - W_0\|_F \leq C \sqrt{\frac{K \log K}{\lambda(C)}}.
\]

(2) After \( t \geq t_0 := \frac{cK \log K}{\eta \lambda(C)} \) iterations where \( \alpha_{\text{max}} = \max_{0 \leq t \leq t_0} \alpha_t \), the entrywise predictions of the learned network with respect to the ground truth labels \( \{y_i\}_{i=1}^n \) satisfy

\[
|f(W_t, x_i) - y_i^*| \leq 4\rho,
\]

for all \( 1 \leq i \leq n \). Furthermore, if the noise level \( \rho \) obeys \( \rho \leq \delta/8 \) the network predicts the correct label for all samples i.e.

\[
\arg \min_{\gamma \in [K]} \| f(W_t, x_i) - \gamma \| = y_i^* \quad \text{for} \quad i = 1, 2, \ldots, n.
\]

See its proof in Appendix D.2.6. This result shows that in the limit \( \epsilon_0 \rightarrow 0 \) where the data points are perfectly clustered, if the width of network and the iterations satisfy \( k \geq C(1 + \psi_1)^2 \Gamma^4 \frac{K \log(K)\| C \|^2}{\lambda(C)^2} \), then our method can exactly recover the ground truth label.

This result can be interpreted as ensuring that the network has enough capacity to fit the cluster centers \( \{c_i\}_{i=1}^K \) and the associated true labels.

Then we consider the perturbed data \( X = [x_1, \ldots, x_n] \) instead of the perfectly clustered data \( \bar{X} = [\bar{x}_1, \ldots, \bar{x}_n] \) obtained by mapping \( x_i \) to its associated cluster center, i.e. \( \bar{x}_i = c_{\ell} \) if \( x_i \) belongs to the \( \ell \)-th cluster. In Theorem 8, we upper bound the parameter distance and output distance under the two kinds of data \( X \) and \( \bar{X} \).

**Theorem 8** (Robustness of gradient path to perturbation). Generate samples \( (x_i, y_i)_{i=1}^n \) according to \( (\rho, \epsilon, \delta) \) corrupted dataset and form the concatenated input/labels \( X \in \mathbb{R}^{d \times n}, y \in \mathbb{R}^n \). Let \( \bar{X} \) be the clean input sample matrix obtained by mapping \( x_i \) to its associated cluster center. Set learning rate \( \eta \leq \frac{K}{2c \epsilon_0 n^2 \| C \|^2} \) and maximum iterations \( t_0 \) satisfying

\[
\eta t_0 = C_1 \frac{K}{\eta n \lambda(C)} \log \left( \frac{\Gamma \sqrt{n} \log K}{\rho} \right),
\]

where \( C_1 \geq 1 \) is a constant of our choice. Suppose input noise level \( \epsilon \) and number of hidden nodes obey

\[
\epsilon \leq O \left( \frac{\lambda(C)}{\Gamma^2 K \log(\frac{\Gamma n \log K}{\rho})} \right) \quad \text{and} \quad k \geq O \left( \frac{\Gamma^{10} K^2 \| C \|^4}{\alpha_{\text{max}}^2 \lambda(C)^4} \log \left( \frac{\Gamma \sqrt{n} \log K}{\rho} \right) \right).
\]


where $\alpha_{\text{max}} = \max_{1 \leq t \leq t_0} \alpha_t$. Assume $2\sqrt{\pi} \sum_{i=0}^{t-1} \left(1 - \frac{i^2}{t^2}\right)^{t-i} |\alpha_t - \alpha_{t+1}| \leq \psi_1 \|r_0\|_2$ and $2\sqrt{\pi} \sum_{i=0}^{t-1} |\alpha_t - \alpha_{t+1}| \leq \psi_1 \|r_0\|_2$. Set $W_0 \sim \mathcal{N}(0,1)$. Starting from $W_0 = \tilde{W}_0$ consider the gradient descent iterations over the losses

$$W_{t+1} = W_t - \eta \nabla L_t(W_t) \quad \text{where} \quad L_t(W) = \frac{1}{2} \sum_{i=1}^{n} (y_{ti} - f(W, x_i))^2$$

and

$$\tilde{W}_{t+1} = \tilde{W}_t - \nabla \tilde{L}_t(\tilde{W}_t) \quad \text{where} \quad \tilde{L}_t(\tilde{W}) = \frac{1}{2} \sum_{i=1}^{n} (\tilde{y}_{ti} - f(\tilde{W}, \tilde{x}_i))^2,$$

Then, for all gradient descent iterations satisfying $t \leq t_0$, we have that

$$\|f(W_t, X) - f(\tilde{W}_t, \tilde{X})\|_2 \leq c_0 \psi' \eta \sqrt{\sqrt{\log K}},$$

and

$$\|W_t - \tilde{W}_t\|_F \leq O \left( t \psi' \eta \frac{K^{1/4} n \log K}{\lambda(C)} \log \left( \frac{\sqrt{n} \log K}{\rho} \right) \right),$$

where $\psi' = 1 + \frac{\psi}{2} + \sqrt{\psi_2}$.

See its proof in Appendix D.2.7. Theorem 2 is obtained by combining the above results together.

**D.2.3 Proof of Theorem 2**

*Proof of Theorem 2.* Here we prove our results by three steps. In these steps, each step proves one of the three results in our theory. To begin with, we consider two parameter update settings with initialization as $W_0$:

$$\tilde{W}_{t+1} = \tilde{W}_t - \nabla \tilde{L}_t(\tilde{W}_t) \quad \text{where} \quad \tilde{L}_t(\tilde{W}) = \frac{1}{2} \sum_{i=1}^{n} (\tilde{y}_{ti} - f(\tilde{W}, \tilde{x}_i))^2,$$

and

$$W_{t+1} = W_t - \eta \nabla L_t(W_t) \quad \text{where} \quad L_t(W) = \frac{1}{2} \sum_{i=1}^{n} (y_{ti} - f(W, x_i))^2,$$

where $\tilde{y}_{ti} = (1 - \alpha_t)y + \alpha_t f(\tilde{W}_t, \tilde{x}_i)$, $y_{ti} = (1 - \alpha_t)y + \alpha_t f(W_t, x_i)$, $\tilde{X} = \{\tilde{x}_1, \ldots, \tilde{x}_n\}$ denotes the clean input sample matrix obtained by mapping $x_i$ to its associated cluster center, i.e. $\tilde{x}_i = c_\ell$ if $x_i$ belongs to the $\ell$-th cluster, and $X = \{x_1, \ldots, x_n\}$ denotes corrupted data matrix. Denote the prediction residual vectors of the noiseless and original problems with respect true ground truth labels $y^*$ by $\tilde{r}_t = f(\tilde{W}_t, \tilde{X}) - y^*$ and $r_t = f(W_t, X) - y^*$ respectively.

Theorem 7 shows that if number of iterations $t$ and network width respectively satisfy $t \geq t_0 := \frac{c\log K}{\eta \lambda(C)} \log \left( \frac{\sqrt{n} \log K}{\alpha \rho} \right)$ and $k \geq C(1 + \psi_1) 2^{1/4} \frac{K \log(K)c^2}{\lambda(C)}$, then it holds

$$\|\tilde{r}_t\|_\infty = \|f(\tilde{W}_t, \tilde{X}) - y^*\|_\infty \leq 4 \rho \quad \text{and} \quad \|\tilde{W}_t - W_0\|_F \leq c_1 \sqrt{K \log K}.\lambda(C).$$

Meanwhile, Theorem 8 proves that if $\varepsilon \leq \mathcal{O} \left( \frac{\lambda(C)}{\Gamma^2 K \log \left( \frac{\sqrt{n} \log K}{\rho} \right)} \right)$ and $k \geq \mathcal{O} \left( \frac{\Gamma^{10} K^2 c^2}{\alpha \max \lambda(C)} \log \left( \frac{\Gamma \sqrt{n} \log K}{\rho} \right)^6 \right)$, then it holds

$$\|\tilde{r}_t - r_t\|_2 \leq \varepsilon \frac{\psi K}{\max \lambda(C)} \log \left( \frac{\Gamma \sqrt{n} \log K}{\rho} \right) \Gamma^3_3 \sqrt{\log K} = \varepsilon \psi' \frac{\Gamma^4 K n \log K}{\lambda(C)} \log \left( \frac{\Gamma \sqrt{n} \log K}{\rho} \right)$$

and

$$\|W_t - \tilde{W}_t\|_F \leq \mathcal{O} \left( t \psi' \eta \frac{K^{1/4} n \log K}{\lambda(C)} \log \left( \frac{\Gamma \sqrt{n} \log K}{\rho} \right)^2 \right),$$

where $\psi' = 1 + \frac{\psi}{2} + \sqrt{\psi_2}$.  

Step 1. By using the above two results, we have
\[ \|f(W_t, X) - \bar{y}\|_2 = \sqrt{n} \|\bar{r}_t\|_2 + \|r_t - \bar{r}_t\|_2 \leq 4\rho + \varepsilon\sqrt{\Gamma^3 K \sqrt{n \log K}} \frac{\log \left( \Gamma \sqrt{n \log K} \right)}{\lambda(C)} \].
Moreover, we can also upper bound
\[ \|\bar{y} - y^*\|_2 \leq \frac{(1 - \alpha_t)\|y - y^*\|_2}{\sqrt{n}} + \frac{\alpha_t\|f(W_t, X) - y^*\|_2}{\sqrt{n}} \]
\[ = \frac{(1 - \alpha_t)\|y - y^*\|_2}{\sqrt{n}} + 4\alpha_t\rho + \varepsilon\sqrt{\Gamma^3 K \sqrt{n \log K}} \frac{\log \left( \Gamma \sqrt{n \log K} \right)}{\rho} \].

Step 2. Now we consider what cases that our method can exactly recover the ground truth label. Assume an input \( x \) is within \( \varepsilon \)-neighborhood of one of the cluster centers \( e \in (e_i)_{i=1}^K \). Then we try to upper bound \( |f(W_t, x) - f(W_t, e)| \) where \( f(W_t, e) \) corresponds to \( f(W_t, \bar{x}) \). To begin with, we have
\[ |f(W_t, x) - f(W_t, e)| \leq |f(W_t, x) - f(W_t, \bar{x})| + |f(W_t, \bar{x}) - f(W_t, e)| \]
We upper bound the first term as follows:
\[ |f(W_t, x) - f(W_t, \bar{x})| = |v^T \phi(W_t x) - v^T \phi(W_t \bar{x})| \leq \|v\|_2 \|\phi(W_t x) - \phi(W_t \bar{x})\|_2 \]
\[ \leq \Gamma \|W_t - \bar{W}\|_F \]
\[ \leq O \left( \varepsilon\sqrt{\Gamma^5 K^2} \frac{\log \left( \Gamma \sqrt{n \log K} \right)}{\lambda(C)^2} \right) \]
where we use the results \( \|W_t - \bar{W}\|_F \leq O \left( \sqrt{\frac{K \log K}{\lambda(C)^2}} \right) \) in Theorem 8, and \( t = t_0 \). Next, we need to bound
\[ |f(W_t, x) - f(W_t, e)| \leq |v^T \phi(W_t x) - v^T \phi(W_t \bar{x})| \]
On the other hand, we have \( \|W_t - W_0\|_F \leq O \left( \Gamma \sqrt{\frac{K \log K}{\lambda(C)^2}} \right) \) in Theorem 7, \( \|x - c\|_2 \leq \varepsilon \) and \( W_0 \sim \mathcal{N}(0, I) \) in assumption. Moreover, using by assumption we have
\[ k \geq O \left( \|W_t - W_0\|_F \right) = O \left( \Gamma^2 \frac{K \log K}{\lambda(C)} \right) \].

By using the above results, Theorem 5 guarantees that with probability at least \( 1 - K \exp(-100d) \), for all inputs \( x \) lying \( \varepsilon \)-neighborhood of cluster centers, it holds that
\[ |f(W_t, x) - f(W_t, \bar{c})| \leq C' \Gamma \varepsilon (\|W_t - W_0\|_F + \sqrt{d}) \leq C \varepsilon \left( \Gamma \sqrt{\frac{K \log K}{\lambda(C)}} + \sqrt{d} \right) \].
Combining the two bounds above we get
\[ |f(W_t, x) - f(W_t, \bar{c})| \leq C \varepsilon \left( \Gamma \sqrt{\frac{K \log K}{\lambda(C)}} \right)^2 \frac{\log \left( \Gamma \sqrt{n \log K} \right)}{\lambda(C)^2} + \Gamma \left( \Gamma \sqrt{\frac{K \log K}{\lambda(C)}} + \sqrt{d} \right) \]
\[ \leq C \varepsilon \left( \frac{\Gamma^5 K^2}{\lambda(C)^2} \frac{\log \left( \Gamma \sqrt{n \log K} \right)}{\lambda(C)^2} + \frac{1}{\varepsilon} \right) \].

Hence, if \( \varepsilon \leq c' \delta \min \left( \frac{\lambda(C)^2}{\varepsilon \varepsilon^5 K^2 \log \left( \Gamma \sqrt{n \log K} \right)} , \frac{1}{\varepsilon} \right) \), we obtain that, for all \( x \), the associated cluster \( \bar{c} \) and true label assigned to cluster \( y^* = y^*(\bar{c}) \), we have that
\[ |f(W_t, x) - y^*| < |f(W_t, \bar{c}) - f(W_t, x)| + |f(W_t, \bar{c}) - y^*| \leq 4\rho + \frac{\delta}{8} \]
Meanwhile, we can upper bound
\[ |y^*_x - y^*_x| \leq (1 - \alpha_t)\|y_x - y^*_x\| + \alpha_t\|f(W_t, x) - y^*_x\| \leq (1 - \alpha_t)\|y_x - y^*_x\| + \alpha_t(4\rho + \frac{\delta}{8}). \]
where \( \hat{y}_t^x = (1 - \alpha_t) y_x + \alpha_t f(W_t, x) \) and \( y_x^* \) respectively denote the estimated label by our label refinery and the ground truth label of sample \( x \). Since \( |y_x - y_x^*| < 1 \), by setting \( 1 \geq \alpha_t \geq 1 - \frac{3}{4} \delta \) and \( \rho \leq \delta/32 \), we have

\[
|\hat{y}_t^x - y_x^*| < \frac{\delta}{2}
\]

This means that for any sample \( x_i \), we have \( |\hat{y}_t^i - y_i^*| < \delta/2 \). Therefore, our label refinery gives the correct estimated labels for all samples. By using the same setting, we obtain

\[
|f(W_t, x) - y^*| < \delta/2.
\]

This means that for any sample \( x_i \), we have \( |f(W_t, x_i) - y_i^*| < \delta/2 \). Therefore, \( W_t \) gives the correct estimated labels for all samples. This competes all proofs.

\[\Box\]

### D.2.4 Proofs of Auxiliary Theories in Appendix D.2

#### D.2.5 Proof of Theorem 6

**Proof.** The proof will be done inductively over the properties of gradient descent iterates and is inspired from the recent work \([28, 29]\). The main difference is that this work uses the label estimation \( \hat{y}^t = (1 - \alpha_t) y + \alpha_t f(w_t) \) and minimizes the squared loss, while both \([28, 29]\) use the corrupted label \( y \) and then minimize the squared loss. By comparison, our method is much more complicated and gives different proofs. Let us introduce the notation related to the residual. Set \( r_t = f(w_t) - \hat{y}^t \) and let \( r_0 = f(w_0) - \hat{y}^0 \) be the initial residual. We keep track of the growth of the residual by partitioning the residual as \( r_t = \tilde{r}_t + \tilde{e}_t \) where

\[
\tilde{e}_t = \mathcal{P}_{S_-}(r_t) \quad , \quad \tilde{r}_t = \mathcal{P}_{S_+}(r_t).
\]

We claim that for all iterations \( t \geq 0 \), the following conditions hold.

\[
\|\tilde{e}_t\|_2 \leq \|\tilde{e}_0\|_2 + \sqrt{\frac{2}{n}} \sum_{i=0}^t |\alpha_i - \alpha_{i+1}| \leq \|\tilde{e}_0\|_2 + \frac{\sqrt{2}}{2} \|r_0\|_2, \quad (21)
\]

\[
\|\tilde{r}_t\|_2 \leq \left(1 - \frac{\eta \alpha^2}{4}\right)^t \|\tilde{r}_0\|_2 + 2\sqrt{n} \sum_{i=0}^{t-1} \left(1 - \frac{\eta \alpha^2}{4}\right)^{t-i} |\alpha_i - \alpha_{i+1}|, \quad (22)
\]

\[
\alpha \frac{4}{t} \||w_t - w_0||_2 + \|\tilde{r}_t\|_2 \leq \|\tilde{r}_0\|_2 + 2\sqrt{n} \sum_{i=0}^t |\alpha_i - \alpha_{i+1}| \leq \|r_0\|_2 + 2\sqrt{n} \sum_{i=0}^t |\alpha_i - \alpha_{i+1}|
\]

\[
\leq (1 + \phi) \|r_0\|_2, \quad (23)
\]

where the last line uses the assumption that \( 2\sqrt{n} \lim_{t \to +\infty} \sum_{i=0}^t \|\alpha_i - \alpha_{i+1}\| \leq \psi_1 ||r_0||_2 \). Assuming these conditions hold, for some \( t > 0 \), inductively, we focus on iteration \( t + 1 \). First, note that these conditions imply that for all \( t \geq i \geq 0 \), \( w_t \in \mathcal{D} \) where \( \mathcal{D} = \{ w \in \mathbb{R}^p \mid ||w - w_0||_2 \leq \frac{4(1 + \psi_1) ||r_0||_2}{\alpha} \} \) is the Euclidian ball around \( w_0 \) of radius \( \frac{4(1 + \psi_1) ||r_0||_2}{\alpha} \). This directly follows from (23) induction hypothesis. Next, we claim that \( w_{t+1} \) is still within the set \( \mathcal{D} \). From Lemma 5, we have that if the results in Eqn. (23) holds, then it holds that

\[
w_{t+1} \in \mathcal{D} = \{ w \in \mathbb{R}^p \mid ||w - w_0||_2 \leq \frac{4(1 + \psi_1) ||r_0||_2}{\alpha} \).
\]

In this way, we can directly use the results in previous lemmas and assumptions. Then we will prove that (22) and (23) hold for \( t + 1 \) as well. Note that, following Lemma 3, gradient descent iterate can be written as

\[
r_{t+1} = (I - \eta G(w_t)) r_t + \hat{y}^t - \hat{y}^{t+1}.
\]
Since both column and row space of $G(w_t)$ is subset of $S_+$, we have that
\[
\hat{e}_{t+1} = \mathcal{P}_{S_-}((I - \eta G(w_t))r_t + \hat{y}^t - \hat{y}^{t+1})
\]
\[
= \mathcal{P}_{S_-}(r_t) + \mathcal{P}_{S_-}(\hat{y}^t - \hat{y}^{t+1})
\]
\[
= \hat{e}_t + \mathcal{P}_{S_-}(\hat{y}^t - \hat{y}^{t+1})
\]
\[
= \hat{e}_t + \sum_{i=0}^t \mathcal{P}_{S_-}(\alpha_{t+1} - \alpha_t)\eta
\]
\[
= \hat{e}_0 + \sum_{i=0}^t \mathcal{P}_{S_-}(\alpha_{t+1} - \alpha_t)\eta
\]
(28)
(29)

So we can upper bound
\[
\|\hat{e}_t\|_2 \leq \|\hat{e}_0\|_2 + 2\sqrt{n} \sum_{i=0}^t |\alpha_i - \alpha_{i+1}| \leq \|\hat{e}_0\|_2 + \psi_1\|r_0\|_2.
\]
(30)

This shows the first statement of the induction. Next, over $S_-$, we have
\[
\hat{r}_{t+1} = \mathcal{P}_{S_+}((I - \eta G(w_t))r_t + \hat{y}^t - \hat{y}^{t+1})
\]
\[
= \mathcal{P}_{S_+}((I - \eta G(w_t))\hat{r}_t) + \mathcal{P}_{S_+}((I - \eta G(w_t))\hat{e}_t) + \mathcal{P}_{S_+}(\hat{y}^t - \hat{y}^{t+1})
\]
\[
= \mathcal{P}_{S_+}((I - \eta G(w_t))\hat{r}_t) + \mathcal{P}_{S_+}(\hat{y}^t - \hat{y}^{t+1})
\]
(31)
(32)
(33)
(34)

where the second line uses the fact that $\hat{e}_t \in S_-$ and last line uses the fact that $\hat{r}_t \in S_+$, in the last line, we let $\hat{y}_t = \mathcal{P}_{S_+}(\hat{y}^t)$. Then we can rewrite $\hat{y}^t - \hat{y}^{t+1}$ as
\[
\hat{y}_t - \hat{y}_{t+1} = (1 - \alpha_t)\eta + \alpha_t f(w_t) - (1 - \alpha_{t+1})\eta + \alpha_{t+1} f(w_{t+1}) = (\alpha_{t+1} - \alpha_t)\eta - (\alpha_{t+1} - \alpha_t) f(w_{t+1}).
\]

At the same time, we can upper bound
\[
\|w_{t+1} - w_t\|_F \leq \eta \|J(w_t)^T r_t\|_2 \leq \eta \|J(w_t)^T \hat{r}_t\|_2 \leq \eta \|\hat{e}_t\|_2.
\]
(35)

In this way, we can obtain
\[
\|\hat{r}_{t+1}\|_2 \leq \|\hat{r}_t\|_2 + \|\eta(\alpha_{t+1} - \alpha_t)\eta\|_2 + \|\alpha_t f(w_t) - f(w_{t+1})\|_2 + \|\alpha_{t+1} f(w_{t+1}) - f(w_{t+1})\|_2
\]
\[
\leq \left(1 - \frac{\eta^2}{2}\right) \|\hat{r}_t\|_2 + \alpha_t \beta \|w_t - w_{t+1}\|_2 + 2\sqrt{n} \cdot |\alpha_t - \alpha_{t+1}|
\]
(36)
\[
\leq \left(1 - \frac{\eta^2}{2}\right) \|\hat{r}_t\|_2 + \alpha_t \beta \|\hat{r}_t\|_2 + 2\sqrt{n} \cdot |\alpha_t - \alpha_{t+1}|
\]
(37)
\[
\leq \left(1 - \frac{\eta^2}{4}\right) \|\hat{r}_t\|_2 + 2\sqrt{n} \cdot |\alpha_t - \alpha_{t+1}|
\]
(38)

where $\hat{e}_t$ uses Lemma 6, $\|\eta\|_2 \leq \sqrt{n}$ and $\|f(w_{t+1})\|_2 \leq \sqrt{n}$, $\hat{r}_t$ uses $\alpha_t \leq \frac{\alpha^2}{4\sigma^2}$. This result further yields
\[
\|\hat{r}_t\|_2 \leq \left(1 - \frac{\eta^2}{4}\right)^t \|\hat{r}_0\|_2 + 2\sqrt{n} \sum_{t=0}^{t-1} \left(1 - \frac{\eta^2}{4}\right)^{t-t} |\alpha_t - \alpha_{t+1}|
\]
(39)

On the other hand, we have
\[
\|\hat{e}_t\|_2 \leq \|\hat{r}_t\|_2 - 2\eta \hat{r}_t^T G(w_t) \hat{r}_t + \eta^2 \hat{r}_t^T G^T(w_t) G(w_t) \hat{r}_t
\]
\[
\leq \|\hat{r}_t\|_2 - 2\eta \hat{r}_t^T J(w_t) J^T(w_t) \hat{r}_t + \eta^2 \beta \|\hat{r}_t\|_2 \|J^T(w_t) \hat{r}_t\|_2
\]
\[
\leq \|\hat{r}_t\|_2 - \eta \|J^T(w_t) \hat{r}_t\|_2,
\]
(40)
(41)
(42)
where the last line use $\eta \leq \frac{1}{\sqrt{n}}$. This further gives
\[
\| (I - \eta G(w_t)) \tilde{r}_t \|_2 \leq \sqrt{\| \hat{r}_t \|_2^2 - \eta \| J^T (w_t) \hat{r}_t \|_2^2} \leq \| \hat{r}_t \|_2 - \eta \| J^T (w_t) \hat{r}_t \|_2^2.
\]
Therefore, we can upper bound $\| \tilde{r}_t \|_2$ in another way which can help to bound $\| w_{t+1} - w_0 \|_2$:

\[
\begin{align*}
\| \tilde{r}_{t+1} \|_2 & \leq \| (I - \eta G(w_t)) \tilde{r}_t \|_2 + \| (\alpha_t - \alpha_{t+1}) y \|_2 + (1 - \alpha_t) \| f(w_t) - f(w_{t+1}) \|_2 + \| (\alpha_{t+1} - \alpha_t) f(w_{t+1}) \|_2 \\
& \leq \| (I - \eta G(w_t)) \tilde{r}_t \|_2 + (1 - \alpha_t) \beta \| w_t - w_{t+1} \|_2 + 2 \sqrt{n} \cdot |\alpha_t - \alpha_{t+1}| \\
& = \| (I - \eta G(w_t)) \tilde{r}_t \|_2 + (1 - \alpha_t) \beta \| J^T (w_t) r_t \|_2 + 2 \sqrt{n} \cdot |\alpha_t - \alpha_{t+1}| \\
& \leq \| \tilde{r}_t \|_2 - \frac{\eta}{2} \| J^T (w_t) \tilde{r}_t \|_2^2 + (1 - \alpha_t) \beta \| J^T (w_t) r_t \|_2 + 2 \sqrt{n} \cdot |\alpha_t - \alpha_{t+1}|.
\end{align*}
\]

Since the distance of $w_{t+1}$ to initial point satisfies:
\[
\| w_{t+1} - w_0 \|_2 \leq \| w_{t+1} - w_t \|_2 + \| w_t - w_0 \|_2 \leq \| w_t - w_0 \|_2 + \eta \| J^T (w_t) r_t \|_2,
\]
we can further bound
\[
\begin{align*}
\frac{\alpha_t}{4} \| w_{t+1} - w_0 \|_2 + \| \tilde{r}_{t+1} \|_2 & \leq \frac{\alpha_t}{4} \left( \| w_{t+1} - w_0 \|_2 + \| \tilde{r}_t \|_2 + \eta \| J^T (w_t) r_t \|_2 \right) + \| \tilde{r}_t \|_2 - \frac{\eta}{2} \| J^T (w_t) \tilde{r}_t \|_2^2 \\
& \quad + (1 - \alpha_t) \beta \| J^T (w_t) r_t \|_2 + 2 \sqrt{n} \cdot |\alpha_t - \alpha_{t+1}| \\
& \leq \frac{\alpha_t}{4} \| w_{t+1} - w_0 \|_2 + \| \tilde{r}_t \|_2 + \frac{\eta}{4} \| J^T (w_t) r_t \|_2 \left( \alpha + 4(1 - \alpha_t) \beta - 2 \frac{\| J^T (w_t) \tilde{r}_t \|_2}{\| \tilde{r}_t \|_2} \right) + 2 \sqrt{n} \cdot |\alpha_t - \alpha_{t+1}| \\
& \leq \frac{\alpha_t}{4} \| w_{t+1} - w_0 \|_2 + \| \tilde{r}_t \|_2 + 2 \sqrt{n} \cdot |\alpha_t - \alpha_{t+1}| \\
& \leq \| \tilde{r}_0 \|_2 + 2 \sqrt{n} \sum_{i=0}^{t} |\alpha_i - \alpha_{i+1}| \leq \| r_0 \|_2 + 2 \sqrt{n} \sum_{i=0}^{t} |\alpha_i - \alpha_{i+1}|,
\end{align*}
\]
where $\odot$ uses $\frac{\| J^T (w_t) \tilde{r}_t \|_2^2}{\| \tilde{r}_t \|_2^2} \geq \alpha$ and $\alpha_t \leq \frac{\alpha_t}{4}$. By setting $t \geq \frac{5}{\eta \alpha^2} \log \left( \frac{\| r_0 \|_2}{(1 - \alpha_{\max}) \nu} \right)$ and $\frac{\eta \alpha^2}{4} \leq \frac{\eta \alpha^2}{4} \leq \frac{1}{8}$ where $\alpha_{\max} = \max_t \alpha_t$, then we have
\[
\log \left( \frac{1 - \frac{\eta \alpha^2}{4}}{1 - \frac{\eta \alpha^2}{4}} \right) \geq \log \left( \frac{1 - \frac{\eta \alpha^2}{4}}{1 - \frac{\eta \alpha^2}{4}} \right) \geq \frac{\eta \alpha^2}{4} \geq \frac{\eta \alpha^2}{4} \quad \text{and thus}
\]
\[
\left( 1 - \frac{\eta \alpha^2}{4} \right)^t \| \tilde{r}_0 \|_2 \leq \left( 1 - \frac{\eta \alpha^2}{4} \right)^t \| r_0 \|_2 \leq \left( 1 - \frac{\eta \alpha^2}{4} \right)^t \| r_0 \|_2 \leq (1 - \alpha_{\max}) \nu.
\]
In this way, we can further obtain
\[
\| \hat{r}_t \|_{\infty} \leq \| \hat{r}_t \|_2 \leq (1 - \alpha_{\max}) \nu + 2 \sqrt{n} \sum_{i=0}^{t-1} \left( 1 - \frac{\eta \alpha^2}{4} \right)^{t-i} |\alpha_i - \alpha_{i+1}|.
\]
and
\[
(1 - \alpha_t) \| P_{S} (f(w_t) - y) \|_{\infty} = \| P_{S} (f(w_t) - (1 - \alpha_t) y - \alpha_t f(w_t)) \|_{\infty} = \| \hat{r}_t \|_{\infty} \leq \| \hat{r}_t \|_2 \\
\leq \| \hat{r}_t \|_2 + \frac{2 \sqrt{n}}{1 - \alpha_t} \sum_{i=0}^{t-1} \left( 1 - \frac{\eta \alpha^2}{4} \right)^{t-i} |\alpha_i - \alpha_{i+1}|.
\]
Finally, we can obtain the desired results:
\[
\begin{align*}
\| f(w_t) - y \|_{\infty} & \leq \| P_{S} (f(w_t)) - P_{S} (y^*) \|_{\infty} \\
& \leq \| P_{S} (f(w_t) - y) \|_{\infty} + \| P_{S} (y - y^*) \|_{\infty} \\
& \leq 2 \nu + \frac{2 \sqrt{n}}{1 - \alpha_t} \sum_{i=0}^{t-1} \left( 1 - \frac{\eta \alpha^2}{4} \right)^{t-i} |\alpha_i - \alpha_{i+1}|.
\end{align*}
\]
where \( \Theta \) holds since \( f(w_t) - y^* \in S_+ \) and \( \|P_{S_+}(f(w_t) - y)\|_\infty = \|P_{S_+}(f(w_t) - y)\|_\infty \). If \( e \) is sparse and \( S_+ \) is diffused, applying Definition 4 we have

\[
\|P_{S_+}(e)\|_\infty \leq \frac{2\sqrt{\alpha}}{n} \|e\|_\infty.
\]

The proof is completed. \( \square \)

**D.2.6 Proof of Theorem 7**

*Proof.* The proof is based on the meta Theorem 6, hence we need to verify its Assumptions 4 and 5 with proper values and apply Lemma 8 to get \( \|P_{S_+}(e)\|_\infty \). We will also make significant use of Corollary 4.

Using Corollary 4, Assumption 5 holds with \( L = \Gamma \sqrt{\frac{\epsilon_{up} n}{kK}} \|C\| \) where \( L \) is the Lipschitz constant of Jacobian spectrum. Denote Using Lemma 7 with probability \( 1 - K^{-100} \), we have that \( \|r_0\|_2 = \|\bar{y}^0 - f(W_0)\|_2 = \|y - f(W_0)\|_2 \leq \Gamma \sqrt{c_0 n \log K} / 128 \) for some \( c_0 > 0 \). Corollary 4 guarantees a uniform bound for \( \beta \), hence in Assumption 4, we pick

\[
\beta \leq \sqrt{\frac{c_{up} n}{K}} \Gamma \|C\|.
\]

We shall also pick the minimum singular value over \( S_+ \) to be

\[
\alpha = \frac{\alpha'}{2} \quad \text{where} \quad \alpha' = \sqrt{\frac{c_{low} n \lambda(C)}{2K}}.
\]

We wish to verify Assumption 4 over the radius of

\[
R = \frac{4\|f(W_0) - y\|_2}{\alpha} \leq \frac{\Gamma \sqrt{c_{low} n \log K / 8}}{\alpha} = \frac{\Gamma \sqrt{c_0 n \log K / 2}}{c_{low} \lambda(C)} = \frac{\Gamma}{c_{low} \lambda(C)}.
\]

neighborhood of \( W_0 \). What remains is ensuring that Jacobian over \( S_+ \) is lower bounded by \( \alpha \). Our choice of \( k \) guarantees that at the initialization, with probability \( 1 - K^{-100} \), we have

\[
\sigma(J(W_0, X), S_+) \geq \alpha'.
\]

Suppose \( LR \leq \alpha = \alpha' / 2 \) which can be achieved by using large \( k \). Using triangle inequality on Jacobian spectrum, for any \( W \in D \), using \( \|W - W_0\|_F \leq R \), we would have

\[
\sigma(J(W, X), S_+) \geq \sigma(J(W_0, X), S_+) - LR \geq \alpha' - \alpha = \alpha.
\]

Now, observe that

\[
LR = (1 + \psi_1) \Gamma \sqrt{\frac{c_{up} n}{kK}} \|C\| \sqrt{c_0 K \log (K)} = (1 + \psi_1) \Gamma^2 \|C\| \sqrt{\frac{c_{up} c_0 n K \log (K)}{c_{low} \lambda(C)}} \tag{35}
\]

\[
\leq \frac{\alpha'}{2} = \sqrt{\frac{c_{low} \lambda(C)}{8K}}, \tag{36}
\]

as \( k \) satisfies

\[
k \geq \mathcal{O} \left((1 + \psi_1)^2 \Gamma^4 \|C\|^2 \frac{c_{up} K \log (K)}{c_{low}^2 \lambda(C)^2}\right) \geq \mathcal{O} \left((1 + \psi_1)^2 \Gamma^4 K \log (K) \|C\|^2 / \lambda(C)^2\right).
\]

Finally, since \( LR = 4(1 + \psi_1) \|r_0\|_2 / \alpha \leq \alpha \), the learning rate is

\[
\eta \leq \frac{1}{2 \beta^2} \min(1, \frac{\alpha \beta}{L \|r_0\|_2}) = \frac{1}{2 \beta^2} \leq \frac{K}{2c_{up} \Gamma^2 \|C\|^2}.
\]

Overall, the assumptions of Theorem 6 holds with stated \( \alpha, \beta, L \) with probability \( 1 - 2K^{-100} \) (union bounding initial residual and minimum singular value events). This implies for all \( t > 0 \) the distance of current iterate to initial obeys

\[
\|W_t - W_0\|_F \leq R.
\]

The final step is the properties of the label corruption. Using Lemma 8, we find that

\[
\|P_{S_+}(y^* - y)\|_\infty \leq 2\rho.
\]
Substituting the values corresponding to $\alpha, \beta, L$ yields that, for all gradient iterations with

$$\frac{5}{\eta n^2} \log \left( \frac{\|r_0\|_2}{2(1 - \alpha_{\max})} \right) \leq \frac{5}{\eta n^2} \log \left( \frac{\sqrt{c_\rho n \log K} / \sqrt{2(1 - \alpha_{\max})}}{\rho} \right) = \mathcal{O} \left( \frac{K}{\eta n \lambda(C)} \log \left( \frac{\sqrt{c_\rho n \log K}}{2(1 - \alpha_{\max}) \rho} \right) \right) \leq t,$$

denoting the clean labels by $\tilde{y}$ and applying Theorem 6, we have that, the infinity norm of the residual obeys (using $\|P_{S_+}(e)\|_\infty = \|P_{S_+}(y - y')\|_\infty \leq 2\rho$)

$$\|f(W) - y^*\|_\infty \leq 4\rho.$$  

This implies that if $\rho \leq \delta/8$, the network will miss the correct label by at most $\delta/2$, hence all labels (including noisy ones) will be correctly classified.  

**D.2.7 Proof of Theorem 8**

**Proof.** Since $\tilde{W}_i$ are the noiseless iterations, with probability $1 - 2K^{-100}$, the statements of Theorem 7 hold on $\tilde{W}_i$. To proceed with proof, we first introduce short hand notations. We use

$$r_i = f(W_i, X) - \tilde{y}^i, \quad \tilde{r}_i = f(\tilde{W}_i, \tilde{X}) - \tilde{y}^i \quad (37)$$

$$J_i = J(W_i, X), \quad J_{i+1,i} = J(W_{i+1}, W_i, X), \quad \tilde{J}_i = J(\tilde{W}_i, \tilde{X}), \quad \tilde{J}_{i+1,i} = J(\tilde{W}_{i+1}, \tilde{W}_i, \tilde{X}) \quad (38)$$

$$d_i = \|W_i - \tilde{W}_i\|_F, \quad p_i = \|r_i - \tilde{r}_i\|_2, \quad \beta = \Gamma\|C\|\sqrt{c_\rho n / K}, \quad L = \Gamma\|C\|\sqrt{c_\rho n / (K\epsilon)}. \quad (39)$$

Here $\beta$ is the upper bound on the Jacobian spectrum and $L$ is the spectral norm Lipschitz constant as in Theorem 4. Applying Lemma 9, note that

$$\|J(W_i, X) - J(\tilde{W}_i, \tilde{X})\| \leq L\|W_i - \tilde{W}_i\|_F + \sqrt{n}\epsilon \leq Ld_i + \sqrt{n}\epsilon \quad (40)$$

$$\|J(W_{i+1}, W_i, X) - J(\tilde{W}_{i+1}, \tilde{W}_i, \tilde{X})\| \leq L(d_i + d_{i+1})/2 + \sqrt{n}\epsilon. \quad (41)$$

By defining

$$\hat{e}_i = P_{S_+}(\tilde{r}_i), \quad \hat{r}_i = P_{S_+}(r_i),$$

then we can use Theorem 6 and the assumption that $2\sqrt{n} \sum_{t=0}^{i-1} \left( 1 - \frac{\alpha^2}{4} \right)^{t-i} |\alpha_t - \alpha_{t+1}| \leq \psi_2 \|r_0\|_2^2$ to obtain

$$\|\hat{e}_i\|_2 \leq \|e_0\|_2 + \sqrt{n} \sum_{t=0}^{i} |\alpha_t - \alpha_{t+1}| \leq \|e_0\|_2 + \frac{\psi_2}{2} \|r_0\|_2, \quad (42)$$

$$\|\hat{r}_i\|_2 \leq \left( 1 - \frac{\alpha^2}{4} \right) \|r_0\|_2 + 2\sqrt{n} \sum_{t=0}^{i-1} \left( 1 - \frac{\alpha^2}{4} \right)^{t-i} |\alpha_t - \alpha_{t+1}| \leq \|r_0\|_2 + \psi_2 \|r_0\|_2. \quad (43)$$

Therefore, we can upper bound

$$\|\hat{r}_i\|_2 = \|\hat{e}_i\|_2 + \|\hat{r}_i\|_2 \leq \|\hat{e}_i\|_2 + \frac{\psi_2}{2} \|r_0\|_2 + \|\hat{r}_i\|_2 + \sqrt{\psi_2} \|r_0\|_2 = \left( 1 + \frac{\psi_2}{2} + \sqrt{\psi_2} \right) \|r_0\|_2. \quad (44)$$

Following this and setting $\|\hat{r}_i\|_2 \leq \psi' \|r_0\|_2$, note that parameter satisfies

$$W_{i+1} = W_i - \eta J_i r_i, \quad \tilde{W}_{i+1} = \tilde{W}_i - \eta \tilde{J}_i \tilde{r}_i \quad (45)$$

$$\|W_{i+1} - \tilde{W}_{i+1}\|_F \leq \|W_i - \tilde{W}_i\|_F + \|\eta\|J_i - \tilde{J}_i\|_{\infty} \|r_i\|_F + \eta\|J_i\|_{\infty} \|r_i - \tilde{r}_i\|_2 \quad (46)$$

$$d_{i+1} \leq d_i + \eta(\psi'(Ld_i + \sqrt{n}\epsilon)) \|r_0\|_2 + \beta p_i, \quad (47)$$

and residual satisfies (using $I \succeq \tilde{J}_{i+1,i} J_i^T / \beta^2 \succeq 0$)

$$r_{i+1} = r_i - \eta J_{i+1,i} J_i^T r_i \iff \quad (48)$$

$$r_{i+1} - \tilde{r}_{i+1} = (r_i - \tilde{r}_i) - \eta (J_{i+1,i} - \tilde{J}_{i+1,i}) J_i^T r_i - \eta \tilde{J}_{i+1,i} J_i^T (r_i - \tilde{r}_i). \quad (49)$$

$$r_{i+1} - \tilde{r}_{i+1} = (I - \eta \tilde{J}_{i+1,i} J_i^T) (r_i - \tilde{r}_i) - \eta (J_{i+1,i} - \tilde{J}_{i+1,i}) J_i^T r_i - \eta \tilde{J}_{i+1,i} (J_i^T - \tilde{J}_i^T) r_i. \quad (50)$$

$$\|r_{i+1} - \tilde{r}_{i+1}\|_2 \leq \|r_i - \tilde{r}_i\|_2 + \eta \beta \|r_i\|_2 (L(3d_i + d_{i+1})/2 + 2\sqrt{n}\epsilon). \quad (51)$$

$$\|r_{i+1} - \tilde{r}_{i+1}\|_2 \leq \|r_i - \tilde{r}_i\|_2 + \eta \beta \|r_i\|_2 (L(3d_i + d_{i+1})/2 + 2\sqrt{n}\epsilon). \quad (52)$$

$$\|r_{i+1} - \tilde{r}_{i+1}\|_2 \leq \|r_i - \tilde{r}_i\|_2 + \eta \beta \|r_i\|_2 (L(3d_i + d_{i+1})/2 + 2\sqrt{n}\epsilon). \quad (53)$$
where we used \( \|r_i\|_2 \leq p_i + \psi'\|r_0\|_2 \) and \( \|(I - \eta(\tilde{T}_{i+1}, \tilde{T}_i^T))v\|_2 \leq \|v\|_2 \) which follows from Lemma 6. This implies

\[
p_{i+1} \leq p_i + \eta \beta(\psi'\|r_0\|_2 + p_i)(L(3d_t + d_{t+1})/2 + 2\Gamma \sqrt{n} \varepsilon).
\]

**Finalizing proof:** Next, using Lemma 7, we have \( \|r_0\|_2 \leq \Theta := C_0 \sqrt{n} \log K \). We claim that if

\[
\varepsilon \leq O\left(\frac{1}{t_0 \eta \Gamma^2 n}\right) \quad \text{and} \quad L \leq \frac{2}{5t_0 \eta \Theta (1 + 8t_0 \eta \beta^2)} \leq \frac{1}{30(t_0 \eta \beta)^2 \Theta}
\]

(where we used \( \eta t_0 \beta^2 \geq 1 \)), for all \( t \leq t_0 \), we have that

\[
p_t \leq 8t(1 + \psi') \eta \Gamma \sqrt{n} \varepsilon \Theta \beta \leq \Theta, \quad d_t \leq 2t \eta \Gamma \sqrt{n} \varepsilon \Theta (\psi' + 8t_0 \eta \beta^2).
\]

The proof is by induction. Suppose it holds until \( t \leq t_0 - 1 \). At \( t + 1 \), via (47) we have that

\[
\frac{d_{t+1} - d_t}{\eta} \leq \psi'(Ld_t \Theta + \Gamma \sqrt{n} \varepsilon \Theta) + 8t_0 \eta \beta^2 \Gamma \sqrt{n} \varepsilon \Theta \leq 2t \sqrt{n} \varepsilon \Theta (\psi' + 8t_0 \eta \beta^2).
\]

Right hand side holds since \( L \leq \frac{1}{\gamma t_0 \Theta} \). This establishes the induction for \( d_{t+1} \).

Next, we show the induction on \( p_t \). Observe that \( 3d_t + d_{t+1} \leq 10t_0 \eta \Gamma \sqrt{n} \varepsilon \Theta (\psi' + 8t_0 \eta \beta^2) \). Following (54) and using \( p_t \leq \Theta \), we need

\[
\frac{p_{i+1} - p_i}{\eta} \leq \beta(1 + \psi') \Theta(L(3d_t + d_{t+1}) + 4\Gamma \sqrt{n} \varepsilon) \leq \frac{8}{\alpha_{\max}}(1 + \psi') \Gamma \sqrt{n} \varepsilon \Theta \beta \iff (57)
\]

\[
L(3d_t + d_{t+1}) + 4\Gamma \sqrt{n} \varepsilon \leq \frac{8}{\alpha_{\max}} \Gamma \sqrt{n} \varepsilon \Theta \iff (58)
\]

\[
L(3d_t + d_{t+1}) \leq \frac{4}{\alpha_{\max}} \Gamma \sqrt{n} \varepsilon \Theta \iff (59)
\]

\[
10\alpha_{\max} L t_0 \eta (1 + 8t_0 \eta \beta^2) \Theta \leq 4 \iff (60)
\]

\[
L \leq \frac{2}{5t_0 \alpha_{\max} \eta (1 + 8t_0 \eta \beta^2) \Theta}, \quad (61)
\]

where \( \alpha_{\max} = \max_{1 \leq t \leq t_0} \alpha_t \). Concluding the induction since \( L \) satisfies the final line. Consequently, for all \( 0 \leq t \leq t_0 \), we have that

\[
p_t = \|r_t - \tilde{r}_t\|_2 = \|f(W_t, X) - \tilde{y}^i - f(\tilde{W}_t, \tilde{X}_i) + \tilde{y}\|_2 \leq \alpha_{\max} \|f(W_t, X) - f(\tilde{W}_t, \tilde{X}_i)\|_2 \leq 8t(1 + \psi') \eta \Gamma \sqrt{n} \varepsilon \Theta = c_0 t(1 + \psi') \eta \Gamma \sqrt{n} \varepsilon \Theta \log K.
\]

where \( \tilde{y}^i = (1 - \alpha_t)y + \alpha_t f(W_t, X) \) and \( \tilde{y}^0 = (1 - \alpha_t)y + \alpha_t f(W_t, \tilde{X}) \). In this way, we can obtain

\[
\|f(W_t, X) - f(\tilde{W}_t, \tilde{X}_i)\|_2 \leq c_0 t(1 + \psi') \eta \Gamma \sqrt{n} \varepsilon \Theta \log K.
\]

Next, note that, condition on \( L \) is implied by

\[
k \geq 1000 \Gamma^2 n (t_0 \eta \beta^2)^2 / \alpha_{\max}^2
\]

\[
= \mathcal{O}\left(\frac{4 \sqrt{n} \Gamma K^2}{\alpha_{\max}^2 \lambda(C)^4} \log\left(\frac{\Gamma \sqrt{n} \log K}{\rho}\right)^4 \right)^{(\|C\|_4^2 (\Gamma \sqrt{n} \log K)^4 (\Gamma \sqrt{n} \log K)^2)}
\]

\[
= \mathcal{O}\left(\frac{\Gamma^{10} K^2 \|C\|_4^4 \log\left(\frac{\Gamma \sqrt{n} \log K}{\rho}\right)^4 \log^2(K)}{\alpha_{\max}^2 \lambda(C)^4} \right)
\]

which is implied by \( k \geq \mathcal{O}\left(\frac{\Gamma^{10} K^2 \|C\|_4^4 \log\left(\frac{\Gamma \sqrt{n} \log K}{\rho}\right)^4 \log^2(K)}{\alpha_{\max}^2 \lambda(C)^4} \right) \).

Finally, following (56), distance satisfies

\[
d_t \leq 20 t \psi' \eta^2 t_0 \Gamma \sqrt{n} \varepsilon \Theta \beta^2 \leq \mathcal{O}\left( t \psi' \eta^2 \frac{\Gamma K n}{\lambda(C)} \log\left(\frac{\Gamma \sqrt{n} \log K}{\rho}\right)^2 \right).
\]

The proof is completed. □